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Chirally improving Wilson fermions

2. Four-quark operators

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ABSTRACT: In this paper we discuss how the peculiar properties of twisted mass lattice QCD at maximal twist can be employed to set up a consistent computational scheme in which, despite the explicit breaking of chiral symmetry induced by the presence of the Wilson and mass terms in the action, it is possible to completely bypass the problem of wrong chirality and parity mixings in the computation of the CP-conserving matrix elements of the $\Delta S = 1, 2$ effective weak hamiltonian, and at the same time have a positive determinant for pairs of non-degenerate quarks, as well as absence of $O(a)$ discretization effects in on-shell quantities with no need of improving lattice action and operators.

KEYWORDS: Lattice Gauge Field Theories, Weak Decays, Lattice QCD.

Contents

1. Introduction	2
2. Sea and valence quarks	4
2.1 Symmetries and renormalization	5
2.2 Sea quark determinant	7
2.3 Renormalization constants and $O(a)$ improvement	8
2.3.1 $O(a)$ improvement via Wilson averaging	9
2.3.2 $O(a)$ improved results from a single simulation	9
2.4 Some conclusive observations	10
3. The B_K parameter	11
3.1 A convenient lattice discretization of $C_{K'QK}$	13
3.2 Proof of the absence of mixing in $Q_{VV+AA}^{\Delta S=2}$	15
4. The $\Delta I = 1/2$ rule from $K \rightarrow \pi\pi$ amplitudes	17
4.1 Kaon decay amplitudes	18
4.2 Correlation functions and valence quarks	18
4.3 A convenient lattice discretization of the $C_{\pm,K\pi\pi}^{(4s10v)}$ correlators	20
4.4 Some observations	21
4.5 The renormalization properties of Q_{VA+AV}^{\pm}	22
4.5.1 Operators of dimension lower than six	22
4.5.2 Operators of dimension six	24
5. The $\Delta I = 1/2$ rule from $K \rightarrow \pi$ amplitudes	25
5.1 Correlation functions and valence quarks	25
5.2 A convenient lattice discretization of the $C_{\pm,K\pi}^{(4s10v)}$ correlators	26
5.3 The renormalization properties of Q_{VV+AA}^{\pm}	27
6. Concluding remarks	28
6.1 Critical mass and $O(a)$ improvement	29
6.2 Tests and numerical issues	30
6.3 Outlook	31
A. Renormalizability of the lattice model (2.1)	31
A.1 Sea quark sector	32
A.2 Valence quark sector	33
A.3 Sea and valence quark mass renormalization	34
B. Isospin and parity breaking effects in the light quark sector	36

C. Absence of the mixing of \mathcal{Q}_{VA+AV}^\pm with operators of dimension six	37
C.1 The operator $\mathcal{Q}_{VA+AV}^{\pm[0]}$	37
C.2 The operator $\mathcal{Q}_{VA+AV}^{\pm[1]}$	38

1. Introduction

In this paper we want to give an explicit set of rules that, within the computational scheme offered by the maximally twisted lattice regularization of QCD [1, 2], allows to extract from simulation data the matrix elements of the CP-conserving part of the $\Delta S = 1, 2$ effective weak hamiltonian ($\mathcal{H}_{\text{eff}}^{\Delta S=1}$ and $\mathcal{H}_{\text{eff}}^{\Delta S=2}$) between pseudo-scalar mesons with no contamination from mixing with operators of wrong chirality or parity, nor $\mathcal{O}(a)$ discretization errors. In contrast, a rather complicated mixing pattern has to be considered in order to construct multiplicatively renormalizable chirally covariant operators if, instead, the standard Wilson fermion regularization is employed [3].

To achieve these remarkable results we will have to treat on different footing internal (sea) and boundary (valence) quark lines. Non-degenerate sea quarks are introduced in pairs and regularized as described in [4]. In this way one gets a real, positive determinant with no vanishing eigenvalues for non-zero values of the quark mass, thus also solving the well known problems with the spectrum of the standard Dirac-Wilson operator. We immediately note that, through quark loops, all lattice quantities at finite a will obviously depend on the set of Wilson parameters, $\{r_p\}$, associated to all the dynamical pairs of quarks ($p = \ell(\text{ight}), h(\text{eavy}), \dots$) present in the action.

As for valence quarks, a precise choice of their flavour structure and regularization scheme has to be made. In this paper we will discuss in detail the case in which valence quarks are introduced à la Österwalder and Seiler [5, 2], but one could equally well imagine to employ fermions obeying the Ginsparg-Wilson (GW) relation [6] for this purpose [7]. In this case $\mathcal{O}(a)$ improvement and no wrong chirality mixing is also achieved, though at the expenses of a fairly larger computational burden compared to what is necessary for the inversion of the standard or twisted Wilson-Dirac fermion operator. It should be immediately observed, however, that the effort to invert, say, the overlap [8, 9] operator is not expected to be larger than that of stochastically evaluating the twisted determinant.

In this paper we want to stick to Wilson-like fermions. We will show that one can still attain the ambitious goals mentioned above within the twisted mass regularization of QCD, with a judicious choice of the structure of the regularized valence quark action. More precisely, we propose to describe each valence flavour, f , with an action of the type

$$\begin{aligned}
S_{\text{OS}}^{(\pi/2)}[q_f, \bar{q}_f, U] &= a^4 \sum_x \bar{q}_f(x) \left[\gamma \cdot \tilde{\nabla} + e^{-i\omega\gamma_5} W_{\text{cr}}(r_f) + m_f \right] \Big|_{\omega=\pi/2} q_f(x) \\
&= a^4 \sum_x \bar{q}_f(x) \left[\gamma \cdot \tilde{\nabla} - i\gamma_5 W_{\text{cr}}(r_f) + m_f \right] q_f(x), \tag{1.1}
\end{aligned}$$

where

$$\gamma \cdot \tilde{\nabla} \equiv \frac{1}{2} \sum_{\mu} \gamma_{\mu} (\nabla_{\mu}^* + \nabla_{\mu}), \quad (1.2)$$

$$W_{\text{cr}}(r_f) \equiv -a \frac{r_f}{2} \sum_{\mu} \nabla_{\mu}^* \nabla_{\mu} + M_{\text{cr}}(r_f), \quad (1.3)$$

with r_f the Wilson parameter for the flavour f and $M_{\text{cr}}(r_f)$ the corresponding critical quark mass. As remarked above, in the full theory $M_{\text{cr}}(r_f)$ also depends on the set of sea quark parameters $\{r_p\}$, though for short we have not indicated this dependence.¹ We will specify below more carefully what is to be meant by “critical mass” in the present context. We wrote the valence quark action in the so-called “physical basis” [2], where m_f is taken to be real (and positive).

The key feature we will exploit in the following is the freedom to regularize each flavour with an appropriately chosen value (of the sign) of the r parameter in front of the corresponding Wilson term.

One might wonder at this point whether the scheme we are proposing is a consistent one, precisely in view of the fact that we are regularizing quarks in different manners according to whether they are sea or valence quarks. It is not difficult to convince oneself that, provided renormalized sea and valence quark masses of the same flavour are made to coincide, this is indeed so. The idea of the argument is to introduce compensating lattice ghost fields (à la Morel [10]) to exactly cancel the fermion determinant of the valence quarks and exploit the symmetries of the extended (local) theory [11] to prove that the Green functions of operators constructed in terms of only ordinary fields have the expected renormalization properties as the lattice spacing, a , is sent to zero (see appendix A for some detail).

We will show that, by replicating some of the valence flavours (and accompanying ghosts) and regularizing them with Wilson terms of suitably chosen signs, the resulting lattice action turns out to have a sufficiently large symmetry so as to imply the cancellation of all the unwanted mixings in the lattice computation of the matrix elements of the CP-conserving $\Delta S = 1$ and $\Delta S = 2$ effective weak hamiltonian. It is important to remark that all these modifications of the lattice action can be made without spoiling the “magic” improvement properties of maximally twisted LQCD [2].

A preliminary study of the scaling properties of maximally twisted LQCD in the quenched approximation has been carried out in ref. [12], where measurements of the pion decay constant and the mass of the vector particle have been performed in the interval $\beta = 5.85 \div 6.2$. Data extrapolate very smoothly to the continuum limit with residual discretization errors consistent with the expected $O(a^2)$ behaviour.

Concluding, we wish to cite the nice paper of ref. [13] in which an interesting step in the direction of alleviating the renormalization problems of the $\mathcal{H}_{\text{eff}}^{\Delta S=1,2}$ operators within the framework of twisted mass LQCD (tm-LQCD) has been taken. The authors show that,

¹Unless differently stated, we employ here the notations of ref. [2]. In particular, the ubiquitous dependence on the bare gauge coupling, g_0^2 , will always be omitted.

with an appropriate choice of the twisting angles of the various flavours, in the computation of $K \rightarrow \pi$ transitions it is possible to remain with at most a linearly divergent counterterm, which in some partially quenched approximation can be even reduced to a finite one.

The plan of the paper is as follows. In section 2 we discuss how valence quarks must be introduced and regularized in order not to lose $O(a)$ improvement and at the same time be ready to get cancellation of wrong chirality and parity mixings in the relevant physical amplitudes. In section 3 we present the strategy for the calculation of B_K , showing how in practice one can get rid of $O(a)$ discretization errors and completely dispose of the contributions potentially coming from the mixing of the bare operator $\mathcal{H}_{\text{eff}}^{\Delta S=2}$ with operators of unwanted chirality and parity. In sections 5 and 4 we extend this procedure to the calculation of the $K \rightarrow \pi$ and $K \rightarrow \pi\pi$ matrix elements of the CP-conserving $\mathcal{H}_{\text{eff}}^{\Delta S=1}$ operator. A few concluding remarks can be found in section 6. Technical details are relegated in some appendices.

2. Sea and valence quarks

In this paper we will consider QCD with four active quark flavours, a situation which represents a rather realistic framework for the computation of the hadronic matrix elements of the effective weak hamiltonian. For the reasons explained in the Introduction we regularize in a different way sea and valence quarks and thus we take the lattice action to be of the form

$$S = S_g[U] + \sum_{p=\ell,h} S_{\text{tm}}^{(\pi/2)}[\psi_p, \bar{\psi}_p, U] + \sum_f \left[S_{\text{OS}}^{(\pi/2)}[q_f, \bar{q}_f, U] + S_{gh}^{(\pi/2)}[\phi_f, U] \right], \quad (2.1)$$

where U are the gauge link variables and $S_g[U]$ stands for any sensible discretization of the pure gauge action. We briefly comment on the three “fermionic” bits of this action.

- Sea quarks ($p = \ell, h$) are arranged in non-degenerate pairs: ψ_ℓ with components $u_{\text{sea}}, d_{\text{sea}}$ (light doublet) and ψ_h with components $s_{\text{sea}}, c_{\text{sea}}$ (heavy doublet). As proposed in ref. [4], they will be described by the maximally twisted action²

$$S_{\text{tm}}^{(\pi/2)}[\psi_p, \bar{\psi}_p, U] = a^4 \sum_x \bar{\psi}_p(x) \left[\gamma \cdot \tilde{\nabla} - i\gamma_5 \tau_1 W_{\text{cr}}(r_p) + m_p - \epsilon_p \tau_3 \right] \psi_p(x) \quad (2.2)$$

with τ_1 and τ_3 acting in flavour space. Integration over the sea quark fields leaves behind a real positive (for $|\epsilon_p| < |m_p|$, $p = \ell, h$) determinant (see ref. [4] and section 2.2).

- Valence quarks are denoted by q_f . Each valence quark will be described by the OS lattice action, $S_{\text{OS}}^{(\pi/2)}[q_f, \bar{q}_f, U]$, specified in eq. (1.1). Since it will turn out to be necessary to introduce “replicas” of the usual u, d, s, c quark fields, we immediately notice that the range of variability of the index f will cover the more extended set of values $u, u', u'', \dots, d, d', d'', \dots, s, s', s'', \dots, c, c', c'', \dots$.

²With respect to ref. [4] we have inverted the sign in front of the mass splitting term.

- In order to have a local representation of correlators with insertion of valence quarks, each q_f will be introduced with an accompanying ghost, ϕ_f , which has the only purpose of exactly canceling the corresponding valence determinant [10]. The action of each ghost reads

$$S_{gh}^{(\pi/2)}[\phi_f, U] = a^4 \sum_x \phi_f^\dagger(x) \text{sign}(m_f) \left[\gamma \cdot \tilde{\nabla} - i\gamma_5 W_{cr}(r_f) + m_f \right] \phi_f(x). \quad (2.3)$$

The (complex) field ϕ_f is an euclidean *commuting* spinor in the fundamental representation of the gauge group with precisely the same value of the mass parameter, m_f , and the same lattice regularization as the quark field, q_f , it corresponds to. Since we will never need to consider correlators with insertions of ghost fields, nor graded field transformations (which turn valence ghosts into valence quarks and viceversa), we do not need to introduce the sophisticated and powerful formalism developed in [11].

The factor “ $\text{sign}(m_f)$ ” in the ghost action (2.3) is inserted in order to guarantee the convergence of the gaussian integral over the ϕ_f field in case $m_f < 0$ [11]. Indeed, with the purpose of discussing renormalizability and $O(a)$ improvement of the correlation functions computed with the action (2.1), in the following we will introduce spurionic symmetries that involve the inversion of the sign of m_f . Thus the case of negative m_f arises, even if one starts with $m_f > 0$.³

As it is formulated, the lattice model with action (2.1) can be viewed as an euclidean statistical theory where the approach of correlation functions to the continuum limit can be discussed on the basis of standard power counting and symmetry arguments. In particular it turns out that renormalized correlation functions admit a well defined continuum limit provided, besides suitably rescaling the bare gauge coupling and setting the critical mass parameters of sea and valence quarks (and corresponding ghosts) to the appropriate values, for each flavour renormalized masses of sea and valence quarks (and ghosts) are given the same numerical value. Actually a continuum limit exists even if renormalized sea and valence quark masses of the same flavour are given different values: however, we will not consider the possibility of partial quenching in this paper.

Energy levels and operator matrix elements of QCD with four quark flavours can be extracted from correlation functions of the model (2.1) with neither ghost nor sea quark fields. As for correlators with sea quark fields, they are also perfectly well defined and are needed, for instance, to compute the renormalization constants Z_P and Z_S (see eq. (2.6) below and appendix A).

2.1 Symmetries and renormalization

Since the lattice regularizations of sea and valence quarks are not identical, implementing the equality of sea and valence renormalized quark masses requires the knowledge of the relation between bare and renormalized masses. Such a relation follows, as usual, from the

³Notice that the factor $\text{sign}(m_f)$ does not introduce any spurious non-analytic behaviour of the ghost determinant in m_f , as its presence only amounts to rescaling the determinant by an overall field-independent factor, which in any case drops out from (connected) correlators.

analysis of the symmetries of the model described by the action (2.1). The result of this analysis, which is presented in appendix A, can be summarized as follows.

- A unique (dimensionless) lattice function, $f_{\text{cr}}(r_1; r_2, r_3)$, exists in terms of which all critical masses can be expressed. Besides the coupling constant (which, as we said, we do not show explicitly), f_{cr} depends on the Wilson parameter, r_1 , of the quark whose critical mass is being considered and on the Wilson parameters of sea quarks. The former — which appears only in the “external” lines of the diagrams relevant for the study of quark mass renormalization — can be r_f , or either r_ℓ or r_h , depending on whether we are dealing with valence or sea quark masses. The further dependence upon the Wilson parameters $r_2 \equiv r_\ell$ and $r_3 \equiv r_h$ is the one that comes from “internal” loops.

In the following for short the dependence on sea quark r -coefficients (r_ℓ and r_h) will always be understood. Thus the relevant formulae for the critical masses will be written in the form

$$\text{sea} \quad aM_{\text{cr}}(r_p) = f_{\text{cr}}(r_p; r_\ell, r_h), \quad p = \ell, h, \quad (2.4)$$

$$\text{valence} \quad aM_{\text{cr}}(r_f) = f_{\text{cr}}(r_f; r_\ell, r_h), \quad \text{all } f' \text{'s}. \quad (2.5)$$

It may be worth noting that also for valence quarks the value of the critical mass is determined by the requirement that $\bar{q}_f \gamma_5 W_{\text{cr}} q_f$ (eq. (1.3)) is a truly dimension five (irrelevant) operator.

- The renormalized quark mass parameters are related to their bare counterparts by the relations

$$\hat{m}_p^\pm = Z_P^{-1}(r_p) m_p \pm Z_S^{-1}(r_p) \epsilon_p, \quad p = \ell, h, \quad (2.6)$$

$$\hat{m}_f = Z_m(r_f) m_f, \quad \text{all } f' \text{'s}, \quad (2.7)$$

where \pm refers to the high and low mass components of each sea quark pair. Also in the above renormalization constants the dependence on the Wilson parameters that enter only through internal loops will be understood in the following. In other words, we will write $Z_I(r)$ as a shorthand for $Z_I(r; r_\ell, r_h)$, $I = m, P, S, \dots$

- $Z_P(r_p)$ and $Z_S(r_p)$ are the renormalization constants of the (non-singlet) sea quark bilinears $\bar{\psi}_p \gamma_5 \tau_{2,3} \psi_p$ and $\bar{\psi}_p \tau_{2,3} \psi_p$, respectively. They can be determined by requiring that the chiral Ward-Takahashi identities (WTI's) of the model (2.1) with insertions of sea quark field operators have the form expected in the corresponding continuum target theory.
- $Z_m(r_f)$ is the inverse renormalization constant of the operator $\bar{q}_f q_f$. The renormalized expression of the latter, in the model we are considering, is $Z_m^{-1}(r_f) [\bar{q}_f q_f + m_f c_{\bar{q}q}(r_f, a m_f) a^{-2}]$, where the dimensionless coefficient $c_{\bar{q}q}$ is even in r_f and $a m_f$.⁴

⁴These properties of $c_{\bar{q}q}$ follow from the spurionic invariances $\mathcal{R}_{5f}^{\text{sp}}$ (eq. (2.16)) and $\mathcal{P}_5 \times (M \rightarrow -M)$ (eqs. (A.9) and (2.12)).

$Z_m(r_f)$ is even in r_f , as it follows, for instance, from the argument given below eq. (2.21), and obeys the relation

$$Z_m(r) \equiv Z_m(r; r_\ell, r_h) = Z_P^{-1}(r; r_\ell, r_h). \quad (2.8)$$

- Conservation of each of the N valence flavour quantum numbers is ensured by the invariance of (2.1) under the $U(1)$ transformations ($f = 1, \dots, N$)

$$\mathcal{I}_f : \begin{cases} q_f(x) \rightarrow e^{i\theta_f} q_f(x), & \bar{q}_f(x) \rightarrow \bar{q}_f(x) e^{-i\theta_f} \\ q_g(x) \rightarrow q_g(x), & \bar{q}_g(x) \rightarrow \bar{q}_g(x) \quad \text{if } g \neq f \end{cases} \quad (2.9)$$

with θ_f a real parameter. Larger vector valence flavour symmetries of course exist if several valence quark species have identical Wilson parameters (and bare masses).

- The flavour singlet axial current $J_{5\mu} = \sum_{f=1}^N \bar{q}_f \gamma_\mu \gamma_5 q_f$, made out of exclusively valence quarks, exhibits the correct anomaly, proportional to N [14].

Generalizing the arguments given in ref. [2], one can prove that $f_{\text{cr}}(r_1; r_2, r_3)$ is odd in r_1 . For instance, if we take $r_1 = r_f$, proving that f_{cr} is odd in its first argument is equivalent to prove that $M_{\text{cr}}(r_f)$ is odd under $r_f \rightarrow -r_f$. This result follows (see appendix A for details) from the observation that under the changes of integration variables

$$\mathcal{R}_{5f} : \begin{cases} q_f(x) \rightarrow q'_f(x) = \gamma_5 q_f(x) \\ \bar{q}_f(x) \rightarrow \bar{q}'_f(x) = -\bar{q}_f(x) \gamma_5 \\ \phi_f(x) \rightarrow \phi'_f(x) = \gamma_5 \phi_f(x) \end{cases} \quad (2.10)$$

the valence quark (plus ghost) action is invariant if we also invert the sign of r_f and m_f [2].

An analogous argument applies if we were to consider the critical mass of sea quarks. In this case one has to perform the change of variables

$$\mathcal{R}_{5p} : \begin{cases} \psi_p(x) \rightarrow \psi'_p(x) = \gamma_5 \psi_p(x) \\ \bar{\psi}_p(x) \rightarrow \bar{\psi}'_p(x) = -\bar{\psi}_p(x) \gamma_5 \end{cases} \quad (2.11)$$

and exploit the fact that for each value of p the fermionic determinant is an even function of the corresponding Wilson parameter, r_p (see section 2.2).

In the following for any $r \in \{r_\ell, r_h; \dots, r_f, \dots\}$ it is understood that $W_{\text{cr}}(r)$ is of the form (1.3) with $M_{\text{cr}}(r)$ the appropriate odd function of r specified in eq. (2.4) or eq. (2.5). We will thus label expectation values by the relevant Wilson parameters $\{r_\ell, r_h; \dots, r_f, \dots\}$ and quark masses $\{m_\ell, \epsilon_\ell, m_h, \epsilon_h; \dots, m_f, \dots\}$, for which we introduce the compact notation

$$M \equiv \{m_f, \text{all } f'\text{'s}; m_p, \epsilon_p, p = \ell, h\}, \quad R \equiv \{r_f, \text{all } f'\text{'s}; r_p, p = \ell, h\}. \quad (2.12)$$

2.2 Sea quark determinant

Integration over sea quark fields gives rise to the product of determinants

$$D = \prod_{p=\ell, h} D_p, \quad (2.13)$$

$$D_p = \text{Det} \left[\gamma \cdot \tilde{\nabla} - i\gamma_5 \tau_1 W_{\text{cr}}(r_p) + m_p - \epsilon_p \tau_3 \right]. \quad (2.14)$$

As proved in [4], each factor in D is even in m_p and ϵ_p . From this result one can show that D_p is also even in r_p . To prove this property we follow again the strategy developed in ref. [2]. By performing in the functional integral that defines D_p the change of variables (2.11), we get the identity

$$\text{Det} \left[\gamma \cdot \tilde{\nabla} - i\gamma_5 \tau_1 W_{\text{cr}}(r_p) + m_p - \epsilon_p \tau_3 \right] = \text{Det} \left[\gamma \cdot \tilde{\nabla} + i\gamma_5 \tau_1 W_{\text{cr}}(r_p) - m_p + \epsilon_p \tau_3 \right]. \quad (2.15)$$

Since D_p is even in m_p and ϵ_p , while $W_{\text{cr}}(r_p)$ is odd in r_p , we get the thesis. It then follows that all the correlators with insertion of operators made out of only valence quark and gluon fields, and thus all the quantities derived from them, are even in r_p , m_p and ϵ_p , $p = \ell, h$. In particular such parity properties imply that $f_{\text{cr}}(r_1; r_2, r_3)$ is an even function of its last two arguments ($r_{2,3} = r_p, p = \ell, h$).

2.3 Renormalization constants and $O(a)$ improvement

The symmetries of the action (2.1) relevant for analyzing the R -dependence of renormalization constants and leading cut-off effects are

- the spurionic $\mathcal{R}_{5f}^{\text{sp}}$ transformation acting on each flavour f separately

$$\mathcal{R}_{5f}^{\text{sp}} \equiv \mathcal{R}_{5f} \times (r_f \rightarrow -r_f) \times (m_f \rightarrow -m_f), \quad (2.16)$$

with \mathcal{R}_{5f} given by eq. (2.10);

- the spurionic $\mathcal{R}_{5p}^{\text{sp}}$ transformation acting on the $p = \ell$ and $p = h$ sea quarks separately,

$$\mathcal{R}_{5p}^{\text{sp}} \equiv \mathcal{R}_{5p} \times (r_p \rightarrow -r_p) \times (m_p \rightarrow -m_p) \times (\epsilon_p \rightarrow -\epsilon_p), \quad (2.17)$$

with \mathcal{R}_{5p} given by eq. (2.11);

- the overall transformation acting on all types of fields

$$\mathcal{D}_d \times \prod_f \mathcal{R}_{5f} \times \prod_{p=\ell, h} \mathcal{R}_{5p} \quad (2.18)$$

with

$$\mathcal{D}_d : \begin{cases} U_\mu(x) \rightarrow U_\mu^\dagger(-x - a\hat{\mu}) \\ \psi_p(x) \rightarrow e^{3i\pi/2} \psi_p(-x), & \bar{\psi}_p(x) \rightarrow e^{3i\pi/2} \bar{\psi}_p(-x), & p = \ell, h \\ q_f(x) \rightarrow e^{3i\pi/2} q_f(-x), & \bar{q}_f(x) \rightarrow e^{3i\pi/2} \bar{q}_f(-x), & \text{all } f\text{'s} \\ \phi_f(x) \rightarrow e^{3i\pi/2} \phi_f(-x), & & \text{all } f\text{'s}. \end{cases} \quad (2.19)$$

We also note the existence of the spurionic symmetry obtained as the product of all invariances of the type (2.16) and (2.17), namely

$$\mathcal{R}^L \times (M \rightarrow -M) \equiv \prod_f \mathcal{R}_{5f} \times \prod_{p=\ell, h} \mathcal{R}_{5p} \times (R \rightarrow -R) \times (M \rightarrow -M). \quad (2.20)$$

Since the formal continuum action we are aiming at, of which (2.1) is the regularized version, will have to be invariant under the (discrete, non-anomalous) spurionic transformation

$$\mathcal{R}^{\text{cont}} \times (M \rightarrow -M) \equiv \prod_f \mathcal{R}_{5f} \times \prod_{p=\ell, h} \mathcal{R}_{5p} \times (M \rightarrow -M), \quad (2.21)$$

it follows that in any renormalization scheme, besides Z_g , the renormalization constants Z_P , Z_S and Z_m , appearing in eqs. (2.6) and (2.7), and those of all the local operators whose bare expression has definite transformation properties under \mathcal{R}^L , will be even functions of R . This is, in fact, necessary for the renormalized operators to behave under the latter transformation as the corresponding bare ones. Furthermore, recalling that the fermionic determinant D_p (eq. (2.14)) is even in r_p , one concludes that all the above renormalization constants will be separately even in (or trivially independent of) r_p , $p = \ell, h$ and r_f , all f 's.

2.3.1 $O(a)$ improvement via Wilson averaging

By a direct generalization of the argument given in ref. [2], the above symmetries and remarks imply that WA 's of expectation values of multiplicatively renormalizable (m.r.), multi-local, gauge invariant operators (with no ghost fields), $O(x_1, x_2, \dots, x_n)$, are $O(a)$ improved, i.e.

$$\begin{aligned} \langle O(x_1, \dots, x_n) \rangle \Big|_{(M)}^{WA} &\equiv \frac{1}{2} \left[\langle O(x_1, \dots, x_n) \rangle \Big|_{(R, M)} + \langle O(x_1, \dots, x_n) \rangle \Big|_{(-R, M)} \right] \\ &= \zeta_O^O(R) \langle O(x_1, \dots, x_n) \rangle \Big|_{(M)}^{\text{cont}} + O(a^2), \end{aligned} \quad (2.22)$$

where it is understood that the space-time arguments x_1, \dots, x_n are at non-zero relative distance in physical units. The multiplicative factor $\zeta_O^O(R)$ is a coefficient (even under $R \rightarrow -R$) whose presence is necessary to match the lattice to the corresponding continuum expectation value.

Analogous results can be derived from eq. (2.22) for energies and operator matrix elements, namely

$$E_{h,n}(\mathbf{k}; R, M) + E_{h,n}(\mathbf{k}; -R, M) = 2E_{h,n}^{\text{cont}}(\mathbf{k}, M) + O(a^2), \quad (2.23)$$

$$\begin{aligned} &\langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(R, M)} + \\ &+ \langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(-R, M)} = 2\zeta_O^O(R) \langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(M)}^{\text{cont}} + O(a^2), \end{aligned} \quad (2.24)$$

where $E_{h,n}(\mathbf{k}; R, M)$ is the energy of $|h, n, \mathbf{k}\rangle \Big|_{(R, M)}$, the n -th eigenstate of the lattice quantum hamiltonian (which we assume to exist) with three-momentum \mathbf{k} and unbroken quantum numbers h , while \mathcal{O} denotes an arbitrary m.r. and gauge invariant local operator.

2.3.2 $O(a)$ improved results from a single simulation

The action (2.1) admits the further spurionic symmetry

$$\mathcal{P} \times (R \rightarrow -R), \quad (2.25)$$

where \mathcal{P} is the parity operation. The latter, with the definition $x_P = (-\mathbf{x}, t)$, has in the present context the form

$$\mathcal{P} : \begin{cases} U_0(x) \rightarrow U_0(x_P), & U_k(x) \rightarrow U_k^\dagger(x_P - a\hat{k}), & k = 1, 2, 3 \\ \psi_p(x) \rightarrow \gamma_0 \psi_p(x_P), & \bar{\psi}_p(x) \rightarrow \bar{\psi}_p(x_P) \gamma_0, & p = \ell, h \\ q_f(x) \rightarrow \gamma_0 q_f(x_P), & \bar{q}_f(x) \rightarrow \bar{q}_f(x_P) \gamma_0, & \text{all } f\text{'s} \\ \phi_f(x) \rightarrow \gamma_0 \phi_f(x_P), & & \text{all } f\text{'s}. \end{cases} \quad (2.26)$$

The spurionic symmetry (2.25) is particularly important, as its existence entails the possibility of associating a definite parity label to m.r. local operators and to eigenstates of the lattice hamiltonian.⁵ By arguments similar to those given in ref. [2] one can prove the validity of the symmetry relations

$$E_{h,n}(\mathbf{k}; -R, M) = E_{h,n}(-\mathbf{k}; R, M), \quad (2.27)$$

$$\langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(-R, M)} = \eta_{hn} \eta_{\mathcal{O}} \eta_{h'n'} \langle h, n, -\mathbf{k} | \mathcal{O} | h', n', -\mathbf{k}' \rangle \Big|_{(R, M)}, \quad (2.28)$$

where $\eta_{\mathcal{O}}$, η_{hn} and $\eta_{h'n'}$ denote the parity labels of the m.r. operator \mathcal{O} and the external states, respectively. Inserting eqs. (2.27) and (2.28) in (2.23) and (2.24), one ends up with the formulae

$$E_{h,n}(\mathbf{k}; R, M) + E_{h,n}(-\mathbf{k}; R, M) = 2E_{h,n}^{\text{cont}}(\mathbf{k}, M) + \mathcal{O}(a^2), \quad (2.29)$$

$$\begin{aligned} & \langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(R, M)} + \\ & + \eta_{hn} \eta_{\mathcal{O}} \eta_{h'n'} \langle h, n, -\mathbf{k} | \mathcal{O} | h', n', -\mathbf{k}' \rangle \Big|_{(R, M)} = 2\zeta_{\mathcal{O}}^{\mathcal{O}}(R) \langle h, n, \mathbf{k} | \mathcal{O} | h', n', \mathbf{k}' \rangle \Big|_{(M)}^{\text{cont}} + \mathcal{O}(a^2), \end{aligned} \quad (2.30)$$

which show that the WA 's (2.23) and (2.24) can be evaluated in terms of correlators and derived quantities obtained from a single simulation with Wilson parameters R .

2.4 Some conclusive observations

It is worth observing that in the lattice model (2.1) the fermionic determinant (2.13) introduces neither lattice artifacts linear in a nor parity breaking effects. This can be seen by considering expectation values of pure gauge (multi-local, gauge invariant) operators, O_{pg} . Such expectation values depend on the sea quark Wilson parameters, r_ℓ and r_h , and are even functions of them, because $D = D_\ell D_h$ is even, but are obviously independent of the valence quark Wilson parameters. We thus have

$$\langle O_{pg}(x_1, \dots, x_n) \rangle \Big|_{(R, M)} = \langle O_{pg}(x_1, \dots, x_n) \rangle \Big|_{(-R, M)}, \quad (2.31)$$

from which, comparing with the WA formula (2.22) written for $O \rightarrow O_{pg}$, we conclude that the expectation values of pure gauge operators trivially coincide with their Wilson average

⁵The assignment of a parity label to eigenstates of the hamiltonian can be done in close analogy with the procedure outlined in sections 5.2 and 5.3 of ref. [2], where the case of twisted mass QCD with one pair of mass degenerate quarks was discussed.

and, hence, are automatically free of $O(a)$ cut-off effects. Moreover, if the operator O_{pg} has a definite parity, $\eta_{O_{pg}} = \pm 1$, i.e. it satisfies the equation

$$\langle O_{pg}(x_1, \dots, x_n) \rangle \Big|_{(R,M)} = \eta_{O_{pg}} \langle O_{pg}(x_{1P}, \dots, x_{nP}) \rangle \Big|_{(-R,M)}, \quad (2.32)$$

then for its expectation value, owing to eq. (2.31), one gets

$$\langle O_{pg}(x_1, \dots, x_n) \rangle \Big|_{(R,M)} = \eta_{O_{pg}} \langle O_{pg}(x_{1P}, \dots, x_{nP}) \rangle \Big|_{(R,M)}, \quad (2.33)$$

which is precisely what one would expect in a parity-invariant theory. In other words, all parity breaking effects in correlators with insertions of valence quark operators (and not containing sea quarks or ghosts) come from the breaking of parity induced by the valence OS quarks themselves, and reduce to $O(a^2)$ in Wilson averaged quantities.

The basic reason behind the validity of these properties is that, as a functional of the set of link variables, $\{U\}$, the (maximally twisted) fermion determinant, $D = D[\{U\}]$, is invariant under the replacement $\{U\} \rightarrow \{U_P\}$, where $\{U_P\}$ is the parity transformed set of link variables. This result can be proved by performing in the functional integral that defines the determinant, D , the change of sea quark integration variables induced by the transformation in the second line of eq. (2.26) and recalling that D is even in $r_p, p = \ell, h$.

All these observations may be of some importance in practice, because they suggest the interesting possibility of employing GW-type fermions to regularize valence quarks and maximally twisted Wilson fermions to describe sea quarks.⁶ In this hybrid framework, whose computational cost does not look prohibitively large on the scale of today's available computer resources, $O(a)$ improvement is automatic. Furthermore, the nice chiral properties of GW fermions are sufficient to ensure absence of all wrong chirality mixings in correlators with insertions of only valence quark and gluon fields.

This last statement might not be obvious. Actually in the next three sections we will show that this remarkable result can be achieved even if valence quarks are regularized à la OS, provided some clever adjustment of the lattice regularization of (four-flavour) QCD and of its computational scheme is made.

3. The B_K parameter

The popular way to discuss the issue of CP violation in the Standard Model is through the study of the compatibility of experimental data with the constraints imposed by the unitarity of the CKM matrix (unitarity triangle) involving the third generation of quark flavours.⁷ One of the key quantity entering this analysis is ϵ_K , which represents the amount of indirect CP-violation in $K \rightarrow \pi\pi$ decay. Exploiting its precise experimental value to constrain the non-trivial vertex of the unitarity triangle requires the knowledge of the parameter B_K .

⁶A very similar proposal, with ordinary (rather than maximally twisted) Wilson fermions playing the role of sea quarks, has been made in ref. [7].

⁷Good reviews on the subject can be found in ref. [15]. For recent summaries of lattice results see the papers quoted in ref. [16].

In the formal continuum euclidean QCD with four quark flavours (u , d , s and c), renormalized at the scale μ , the kaon B -parameter, $B_K(\mu)$, is defined by the formula

$$\langle \bar{K}^0 | \hat{\mathcal{O}}_{VV+AA}^{\Delta S=2}(\mu) | K^0 \rangle = \frac{16}{3} M_K^2 F_K^2 B_K(\mu). \quad (3.1)$$

B_K can be extracted from the correlator ($x_0 > 0$, $y_0 < 0$)

$$C_{K\mathcal{O}K}^{(\text{qcd4})}(x, y) = \langle (\bar{d}\gamma_5 s)(x) \hat{\mathcal{O}}_{VV+AA}^{\Delta S=2}(0) (\bar{d}\gamma_5 s)(y) \rangle, \quad (3.2)$$

where the bare expression of the renormalized operator $\hat{\mathcal{O}}_{VV+AA}^{\Delta S=2}$ is

$$\mathcal{O}_{VV+AA}^{\Delta S=2} = (\bar{s}\gamma_\mu d)(\bar{s}\gamma_\mu d) + (\bar{s}\gamma_\mu \gamma_5 d)(\bar{s}\gamma_\mu \gamma_5 d) \quad (3.3)$$

and the superscript (qcd4) denotes QCD with four quark species.

We want to show that it is possible to set up a lattice regularization based on (twisted) Wilson fermions, where B_K can be computed in terms of a four-quark operator which does not mix with any other operator of the theory.

In order to explain our strategy it is convenient to first consider at a formal level an auxiliary gauge model where, besides the four lightest sea quark flavours (u_{sea} , d_{sea} , s_{sea} and c_{sea}), each of the d and s valence quark species is duplicated. The valence quarks u , d , d' , s , s' and c are introduced together with the corresponding ghosts, required to cancel the associated valence determinant. We will denote the correlators of this model by the superscript (4s6v). It is not difficult to convince oneself that in this model the correlator

$$C_{K'\mathcal{Q}K}^{(4s6v)}(x, y) = \langle (\bar{d}'\gamma_5 s')(x) 2\mathcal{Q}_{VV+AA}^{\Delta S=2}(0) (\bar{d}\gamma_5 s)(y) \rangle, \quad (3.4)$$

where⁸

$$\begin{aligned} \mathcal{Q}_{VV+AA}^{\Delta S=2} = & (\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu d') + (\bar{s}\gamma_\mu \gamma_5 d)(\bar{s}'\gamma_\mu \gamma_5 d') + \\ & + (\bar{s}\gamma_\mu d')(\bar{s}'\gamma_\mu d) + (\bar{s}\gamma_\mu \gamma_5 d')(\bar{s}'\gamma_\mu \gamma_5 d), \end{aligned} \quad (3.5)$$

contains the same physical information as the “target” correlator $C_{K\mathcal{O}K}^{(\text{qcd4})}(x, y)$ in four-flavour QCD.

To see this we simply have to imagine to have regularized the two models in the same way, for instance, by using GW fermions for all quark fields. If the bare masses of the quarks of the same flavour are given the same value, i.e. if one sets

$$\begin{aligned} m_u^{(\text{qcd4})} = m_u^{(4s6v)} = m_{u_{\text{sea}}}^{(4s6v)}, & \quad m_d^{(\text{qcd4})} = m_d^{(4s6v)} = m_{d'}^{(4s6v)} = m_{d_{\text{sea}}}^{(4s6v)}, \\ m_c^{(\text{qcd4})} = m_c^{(4s6v)} = m_{c_{\text{sea}}}^{(4s6v)}, & \quad m_s^{(\text{qcd4})} = m_s^{(4s6v)} = m_{s'}^{(4s6v)} = m_{s_{\text{sea}}}^{(4s6v)}, \end{aligned} \quad (3.6)$$

then by an elementary application of the Wick theorem one checks that the equality

$$C_{K'\mathcal{Q}K}^{(4s6v)}(x, y) = C_{K\mathcal{O}K}^{(\text{qcd4})}(x, y) \quad (3.7)$$

holds (sea quark loops trivially contribute the same to the two sides of the relation) for any value of the lattice spacing. This result implies that the two operators, $\mathcal{O}_{VV+AA}^{\Delta S=2}$

⁸What we really mean with the superscript $\Delta S = 2$ in $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ is $\Delta s + \Delta s' = 2$.

in the (qcd4) model and $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ in the (4s6v) model, can be taken to have the same renormalization constants. The same is also true for the renormalization constants of the operator $\bar{d}\gamma_5 s$ in the (qcd4) model and the operators $\bar{d}\gamma_5 s$ and $\bar{d}'\gamma_5 s'$ in the (4s6v) model. Moreover, it is obvious that the renormalized masses of the quarks of the same flavour are (can be chosen to be) equal in the two models. With this natural choice of renormalization conditions, the relation (3.7) holds for the corresponding renormalized correlators and carries over to the continuum limit.

The strategy we propose for the evaluation of B_K is based on eq. (3.7) and consists in considering the correlator $C_{K'QK}^{(4s6v)}(x, y)$ in the UV regularization provided by the maximally twisted action (2.1). The reason for selecting this UV regularization is that, with a careful choice of the Wilson parameters of valence quarks, $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ will not mix with any other operator of the theory.

3.1 A convenient lattice discretization of $C_{K'QK}$

In view of the previous remarks, we are led to consider the lattice regularized gauge model (2.1) with valence quarks $q_u \equiv u$, $q_d \equiv d$, $q_{d'} \equiv d'$, $q_s \equiv s$, $q_{s'} \equiv s'$ and $q_c = c$, each having an action of the form (1.1) (accompanied by the corresponding ghosts, $\phi_u, \phi_d, \phi_{d'}, \phi_s, \phi_{s'}, \phi_c$) plus two sea quark doublets, $\psi_\ell \equiv (u_{\text{sea}}, d_{\text{sea}})$ and $\psi_h \equiv (s_{\text{sea}}, c_{\text{sea}})$. The details of the lattice formulation of this theory are as explained in general in section 2. We will refer to this regularized theory as the $(4s6v)_{tm}^L$ model.

For reasons that will become soon clear we take the Wilson parameters of the valence down and strange fields to be related in the following way⁹

$$r_d = r_s = r_{d'} = -r_{s'}. \quad (3.8)$$

Obviously, in order to obtain from the $(4s6v)_{tm}^L$ model correlators that in the continuum limit are equal to those of four-flavour euclidean QCD, we must require the renormalized masses of the (sea and valence) quarks of the same flavour to take identical values, i.e.¹⁰

$$\begin{aligned} \hat{m}_\ell^- &= \hat{m}_u, & \hat{m}_\ell^+ &= \hat{m}_d = \hat{m}_{d'}, \\ \hat{m}_h^- &= \hat{m}_s = \hat{m}_{s'}, & \hat{m}_h^+ &= \hat{m}_c, \end{aligned} \quad (3.9)$$

and be equal to those of the target theory, (qcd4). In terms of bare masses, while the conditions $\hat{m}_d = \hat{m}_{d'}$ and $\hat{m}_s = \hat{m}_{s'}$ are satisfied (owing to eqs. (2.7) and (3.8) and the fact that $Z_m(r_f)$ is even in r_f) by simply setting

$$m_{d'} = m_d, \quad m_{s'} = m_s, \quad (3.10)$$

the remaining four conditions in eq. (3.9) imply a non-trivial one-to-one correspondence between m_u, m_d, m_s, m_c and the sea quark bare mass parameters $m_\ell, \epsilon_\ell, m_h, \epsilon_h$, as dictated by eqs. (2.6)–(2.7).

⁹Other equivalent choices, like $r_d = r_s = -r_{d'} = r_{s'}$ are possible. All the arguments we give in this section can be immediately adapted to these other cases.

¹⁰Our notation is such that e.g. $m_\ell^+ = m_{d_{\text{sea}}}$ and $m_h^- = m_{s_{\text{sea}}}$.

We now prove that in the lattice model $(4s6v)_{tm}^L$, with the set of quark masses, M , satisfying the conditions (3.9), the (bare) B_K parameter can be extracted from the correlator

$$a^6 \sum_{\mathbf{x}, \mathbf{y}} C_{K' \mathcal{Q}K}^{(4s6v)_{tm}^L}(x, y) = a^6 \sum_{\mathbf{x}, \mathbf{y}} \langle (\bar{d}' \gamma_5 s')(x) 2\mathcal{Q}_{VV+AA}^{\Delta S=2}(0) (\bar{d} \gamma_5 s)(y) \rangle \Big|_{(R, M)}, \quad (3.11)$$

with the operator $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ given in eq. (3.5) and the (m.r.) pseudo-scalar $(\bar{d}' \gamma_5 s')$ and $(\bar{d} \gamma_5 s)$ densities¹¹ playing the role of interpolating fields for the K^0 and \bar{K}^0 states. The proof is divided in two parts. We first show how B_K is related to the large time behaviour of the correlator (3.11) and in the next section we prove that the operator (3.5) does not mix with any other operator with the same unbroken quantum numbers. A similar result was already derived within the standard tm-LQCD approach of ref. [1] and exploited in ref. [17] in actual simulations. In the present scheme one gets two extra bonuses: an automatically $O(a)$ improved determination of B_K (as it follows from the arguments we give at the end of this section) and a positive definite fermion determinant even in the mass non-degenerate case [4].

On a lattice with very large temporal extension the leading contribution to the spectral representation of the correlator (3.11) in the $(4s6v)_{tm}^L$ theory is given by

$$\frac{e^{-M_{K'}|x_0| - M_K|y_0|}}{4M_{K'}M_K} \langle \Omega | \bar{d}' \gamma_5 s' | \bar{K}'^0 \rangle \langle \bar{K}'^0 | 2\mathcal{Q}_{VV+AA}^{\Delta S=2} | K^0 \rangle \langle K^0 | \bar{d} \gamma_5 s | \Omega \rangle \Big|_{(R, M)}, \quad (3.12)$$

where K^0 (\bar{K}'^0) is the neutral kaon (anti-kaon) state created from the vacuum Ω by the operator $-\bar{d} \gamma_5 s$ ($\bar{s}' \gamma_5 d'$) and M_K ($M_{K'}$) the corresponding meson mass. We remark that with the choice (3.8) of the (valence) Wilson parameters, the lattice kaon mass, M_K , and kaon decay constant, F_K , defined in terms of the valence quark fields d and s may differ by $O(a^2)$ effects from their counterparts, $M_{K'}$ and $F_{K'}$, analogously defined in terms of the twin valence quarks d' and s' . Keeping track of this difference, we write the relation which defines the bare B_K parameter in the form

$$\langle \bar{K}'^0 | 2\mathcal{Q}_{VV+AA}^{\Delta S=2} | K^0 \rangle = \frac{16}{3} M_{K'} F_{K'} M_K F_K B_K^{\text{bare}}. \quad (3.13)$$

The values of M_K , F_K , $M_{K'}$ and $F_{K'}$ can be obtained in the usual way from the study of the two-point correlation functions

$$a^3 \sum_{\mathbf{x}} \langle (\bar{s} \gamma_5 d)(0) (\bar{d} \gamma_0 \gamma_5 s)(x) \rangle, \quad a^3 \sum_{\mathbf{x}} \langle (\bar{s}' \gamma_5 d')(0) (\bar{d}' \gamma_0 \gamma_5 s')(x) \rangle. \quad (3.14)$$

The renormalized B_K parameter is finally given by

$$B_K(\mu) = Z_{\mathcal{Q}_{VV+AA}^{\Delta S=2}}(a\mu) B_K^{\text{bare}}, \quad (3.15)$$

with $Z_{\mathcal{Q}_{VV+AA}^{\Delta S=2}}$ the renormalization constant of $\mathcal{Q}_{VV+AA}^{\Delta S=2}$.

¹¹Mixing of $(\bar{d}' \gamma_5 s')$ with $(\bar{d}' s')$ and of $(\bar{d} \gamma_5 s)$ with $(\bar{d} s)$ is ruled out by the invariance of the lattice model under $\mathcal{P}_5 \times (M \rightarrow -M)$, where \mathcal{P}_5 is defined in eq. (A.9). More precisely these are $O(a)$ effects that appear with coefficients proportional to $a(m_s + m_d)$ or $a(m_s - m_d)$.

The correlation function (3.11) can be $O(a)$ improved via WA , according to the prescription (2.22), and the same holds for all masses and matrix elements that occur in its spectral representation. However, this is not necessary. In fact, thanks to the spurionic symmetry (2.25), M_K , $M_{K'}$, F_K and $F_{K'}$ (see eqs. (2.29) and (2.30)), as well as all the quantities that can be extracted from the correlator (3.11), are automatically free of $O(a)$ cut-off effects. This property follows from the fact that (3.11) is the expectation value of a m.r. operator with the insertion of two other operators taken at vanishing spatial three-momentum. Consequently, B_K^{bare} as defined above can be extracted from automatically $O(a)$ improved data. The same is true for the renormalization constant of the operator $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ (see section 3.3 of ref. [2] and section 2.3.2 of this paper).

3.2 Proof of the absence of mixing in $\mathcal{Q}_{VV+AA}^{\Delta S=2}$

Absence of wrong chirality and parity mixing in the (renormalizable expression of the) operator $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ is proved relying on the symmetries of the lattice model (2.1) supplemented by the specifications given in section 3.1. In particular the conditions (3.8) and (3.10) are assumed to be fulfilled.

It is almost obvious that the operator $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ can not mix with operators of dimension less than six, because of its flavour structure and the fact that the valence sector of the action (2.1) is diagonal in flavour. In particular, the valence flavour quantum numbers d , d' , s and s' are all conserved, as it formally follows from the invariance of the action under the four $U(1)$'s vector transformations, \mathcal{I}_f , $f = d, d', s, s'$, of eq. (2.9). We conclude that $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ can only mix with four fermion operators with $\Delta s = \Delta s' = 1$ and $\Delta d = \Delta d' = -1$.

In order to rule out mixing with other six-dimensional operators satisfying the above selection rules, one must use the following extra symmetries enjoyed by the model action we are considering, i.e.

1. $\text{Ex}(d, d') \times (m_d \leftrightarrow m_{d'})$,
2. $\text{Ex}_5(s, s') \times (m_s \leftrightarrow -m_{s'})$,
3. $\mathcal{C} \times [\text{Ex}(d, s) \times (m_d \leftrightarrow m_s)] \times [\text{Ex}_5(d', s') \times (m_{d'} \leftrightarrow -m_{s'})]$,
4. $\mathcal{P}_5 \times (M \rightarrow -M)$,

where \mathcal{C} and \mathcal{P}_5 are defined in eqs. (A.1) and (A.9) of appendix A, respectively, and

$$\text{Ex}(f_1, f_2) : \quad q_{f_1} \leftrightarrow q_{f_2} \quad \bar{q}_{f_1} \leftrightarrow \bar{q}_{f_2} \quad \phi_{f_1} \leftrightarrow \phi_{f_2}, \quad (3.16)$$

$$\text{Ex}_5(f_1, f_2) : \quad \begin{cases} q_{f_1} \rightarrow \gamma_5 q_{f_2} & \bar{q}_{f_1} \rightarrow -\bar{q}_{f_2} \gamma_5 & \phi_{f_2} \rightarrow \gamma_5 \phi_{f_1} \\ q_{f_2} \rightarrow \gamma_5 q_{f_1} & \bar{q}_{f_2} \rightarrow -\bar{q}_{f_1} \gamma_5 & \phi_{f_1} \rightarrow \gamma_5 \phi_{f_2} \end{cases} \quad (3.17)$$

The transformation $\text{Ex}(f_1, f_2)$ simply represents the exchange of valence flavours f_1 and f_2 with its action appropriately extended to ghost fields. The transformation $\text{Ex}_5(f_1, f_2)$ is nothing but the product

$$\text{Ex}_5(f_1, f_2) = \text{Ex}(f_1, f_2) \times \mathcal{R}_{5f_1} \times \mathcal{R}_{5f_2}. \quad (3.18)$$

Notice that, if $r_{f_1} = r_{f_2}$, $\text{Ex}(f_1, f_2)$ is a symmetry of the action (2.1) when combined with $(m_{f_1} \rightarrow m_{f_2})$. If instead $r_{f_1} = -r_{f_2}$, the action is invariant under $\text{Ex}_5(f_1, f_2) \times (m_{f_1} \leftrightarrow -m_{f_2})$.

Symmetry 1 rules out the dimension six operators that, besides obeying the selection rules $\Delta s = \Delta s' = -\Delta d = -\Delta d' = 1$, are not even under $\text{Ex}(d, d')$. A basis of operators with the desired unbroken quantum numbers is provided by $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ itself and the operators [18, 19] that, with obvious notations, we list below

$$\begin{aligned} \mathcal{Q}_{VV-AA}^{\Delta S=2}, \quad \mathcal{Q}_{SS\pm PP}^{\Delta S=2}, \quad \mathcal{Q}_{TT}^{\Delta S=2}, \\ \mathcal{Q}_{VA\pm AV}^{\Delta S=2}, \quad \mathcal{Q}_{SP\pm PS}^{\Delta S=2}, \quad \mathcal{Q}_{T\bar{T}}^{\Delta S=2}. \end{aligned} \quad (3.19)$$

For instance, we have $(\sigma_{\mu\nu} \equiv i[\gamma_\mu, \gamma_\nu]/2)$

$$\begin{aligned} \mathcal{Q}_{VA\pm AV}^{\Delta S=2} = (\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu\gamma_5 d') \pm (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}'\gamma_\mu d') + \\ + (\bar{s}\gamma_\mu d')(\bar{s}'\gamma_\mu\gamma_5 d) \pm (\bar{s}\gamma_\mu\gamma_5 d')(\bar{s}'\gamma_\mu d), \end{aligned} \quad (3.20)$$

$$\mathcal{Q}_{T\bar{T}}^{\Delta S=2} = \epsilon_{\mu\nu\lambda\rho} [(\bar{s}\sigma_{\mu\nu} d)(\bar{s}'\sigma_{\lambda\rho} d') + (\bar{s}\sigma_{\mu\nu} d')(\bar{s}'\sigma_{\lambda\rho} d)]. \quad (3.21)$$

None of the (dimension six) operators in (3.19) can mix with $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ thanks to the other three (spurionic) symmetries introduced above. In fact

- symmetry 2 rules out $\mathcal{Q}_{VV-AA}^{\Delta S=2}$ and $\mathcal{Q}_{SS-PP}^{\Delta S=2}$ (the latter are odd, while $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ is even);
- symmetry 3 rules out $\mathcal{Q}_{TT}^{\Delta S=2}$ and $\mathcal{Q}_{SS+PP}^{\Delta S=2}$ (the latter are odd, while $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ is even);
- symmetry 4 rules out $\mathcal{Q}_{VA\pm AV}^{\Delta S=2}$, $\mathcal{Q}_{SP\pm PS}^{\Delta S=2}$ and $\mathcal{Q}_{T\bar{T}}^{\Delta S=2}$ (the latter are odd, while $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ is even).

The symmetries we have employed to exclude mixing of $\mathcal{Q}_{VV+AA}^{\Delta S=2}$ with the operators (3.19) can be viewed as the analog of the usual (spurionic) CPS symmetry [19] translated in the present chirally twisted lattice framework. Indeed, if valence quark (and ghost) fields are rotated to the basis where the (subtracted) Wilson term appears in the standard (untwisted) form, while the mass term is chirally twisted, the spurionic symmetry obtained by combining the transformations 3 and 4 above turns out to correspond to the CPS invariance of the standard Wilson theory.

We conclude this section by observing that the whole argument about the absence of mixing in the operator entering the matrix element from which B_K is extracted could be repeated by duplicating only the valence strange quark, and not the down quark. If one does so, one also has to change the form of the operator in eq. (3.5) with the substitution

$$\mathcal{Q}_{VV+AA}^{\Delta S=2} \rightarrow (\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu d) + (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}'\gamma_\mu\gamma_5 d) \quad (3.22)$$

and accordingly modify the expression of the interpolating field of K'_0 from $\bar{d}'\gamma_5 s'$ to $\bar{d}\gamma_5 s'$. The reason why this is possible lies in the observation that, given eqs. (3.8) and (3.10),

the flavour d' is actually indistinguishable from d .¹² In section 3.2 we have presented the line of arguments leading to absence of mixing in the apparently more complicated setting where also the down quark is replicated, because it turns out that in this way the proof goes through in a somewhat simpler fashion.

4. The $\Delta I = 1/2$ rule from $K \rightarrow \pi\pi$ amplitudes

A long standing puzzle in low energy particle physics, often referred to as “octet enhancement” or the $\Delta I = 1/2$ rule [20], is represented by the surprisingly large experimental value of the ratio

$$R(K \rightarrow \pi\pi) = \frac{\Gamma(K \rightarrow \pi\pi)|_{\Delta I=1/2}}{\Gamma(K \rightarrow \pi\pi)|_{\Delta I=3/2}} \sim 400. \quad (4.1)$$

Although the rate of the $\Delta I = 3/2$ $K \rightarrow \pi\pi$ weak decays can be reasonably well computed within our present understanding of field theory (based on O.P.E. and renormalization group arguments), theoretical estimates of the $\Delta I = 1/2$ amplitude seem to give a much too small value compared to the experimental number [21].

Due to the amount of seemingly well founded theoretical ideas involved in this calculation, it is a crucial question to understand whether this discrepancy is due to our ignorance of non-perturbative QCD effects in the hadronic matrix elements of the composite quark operators appearing in the effective weak hamiltonian, or whether this problem should be rather taken as an indication of the existence of some kind of new physics waiting to be uncovered in kaon phenomenology. Lattice gauge theory represents the ideal framework in which this question should find an answer. There are, however, severe technical and conceptual difficulties in the process of establishing the proper strategy to accomplish this task.

First of all, when working with euclidean metric, as one always does in lattice simulations, the procedure necessary to extract the kaon decay amplitudes of physical interest is complicated by IR subtleties arising from final (two-pion) state interactions [22]. To attack this problem new interesting ideas have been recently put forward [23, 24]. Here we will not be concerned with such delicate issues.

The main objective of this paper is rather to deal with the UV difficulties related to the construction of the renormalized effective weak hamiltonian operator on the lattice. We will show that tm-LQCD at maximal twist offers a computational scheme in which the problem of wrong chirality mixing, which afflicts the approach based on standard Wilson fermions [3, 25],¹³ is completely absent. An important step in this direction is represented by the recent paper of ref. [13], where the problem of mixing has been brought to an amenable solution. Here we prove that the calculation can be carried out in a fully $O(a)$ improved way without the need of introducing the Sheikholeslami-Wohlert [28] term in the lattice action, or improving the lattice operators [29, 30] representing the CP-conserving effective weak hamiltonian, while still having a positive definite determinant even for non-degenerate quarks.

¹²We thank D. Bećirević for drawing our attention on this point.

¹³See, however, ref. [26] for some way-outs if the Wilson theory is fully $O(a)$ improved à la Symanzik [27, 28, 29, 30].

4.1 Kaon decay amplitudes

In the Standard Model the decay of the K meson into pion states is described to leading order in the Fermi constant, G_F , by the CP-conserving, $\Delta S = 1$ effective weak hamiltonian, which (in the chiral limit) reads [20]

$$\mathcal{H}_{\text{eff}}^{\Delta S=1} = V_{ud}V_{us}^* \frac{G_F}{\sqrt{2}} \left[C_+ \left(\frac{\mu}{M_W} \right) \hat{\mathcal{O}}^+(\mu) + C_- \left(\frac{\mu}{M_W} \right) \hat{\mathcal{O}}^-(\mu) \right], \quad (4.2)$$

where $V_{ud}V_{us}^*$ is the product of the appropriate matrix elements of the CKM matrix.¹⁴ The effective operator $\mathcal{H}_{\text{eff}}^{\Delta S=1}$ is obtained after having integrated out all degrees of freedom above some energy scale, Λ , with Λ larger than the charm threshold, but still well below the W-boson mass, M_W . Consistently, the operators $\hat{\mathcal{O}}^\pm$ in eq. (4.2) are renormalized at the scale μ with $m_c \ll \mu \ll M_W$, and the Wilson coefficients $C_\pm(\mu/M_W)$ carry the information about the physics between μ and M_W . The expression of the bare operators corresponding to $\hat{\mathcal{O}}^\pm$ is

$$\mathcal{O}^\pm = \frac{1}{2} \left[(\bar{s}\gamma_\mu^L u)(\bar{u}\gamma_\mu^L d) \pm (\bar{s}\gamma_\mu^L d)(\bar{u}\gamma_\mu^L u) \right] - \frac{1}{2} [u \leftrightarrow c] \quad (4.3)$$

with $\gamma_\mu^L = \gamma_\mu(1 - \gamma_5)$.

For the purpose of making contact with experimental data it is enough to consider the decay of the neutral kaon, K^0 , into either $\pi^+\pi^-$ or $\pi^0\pi^0$ states [19, 31, 32, 13]. Owing to the parity invariance of the *formal* continuum QCD, the relevant amplitudes

$$\mathcal{A}_{K^0 \rightarrow \pi^+\pi^-} = V_{ud}V_{us}^* \frac{G_F}{\sqrt{2}} \sum_{j=+,-} C_j \left(\frac{\mu}{M_W} \right) \langle \pi^+\pi^- | \hat{\mathcal{O}}_{V A+AV}^j(\mu) | K^0 \rangle, \quad (4.4)$$

$$\mathcal{A}_{K^0 \rightarrow \pi^0\pi^0} = V_{ud}V_{us}^* \frac{G_F}{\sqrt{2}} \sum_{j=+,-} C_j \left(\frac{\mu}{M_W} \right) \langle \pi^0\pi^0 | \hat{\mathcal{O}}_{V A+AV}^j(\mu) | K^0 \rangle, \quad (4.5)$$

can be written in terms of matrix elements of renormalized parity odd operators, $\hat{\mathcal{O}}_{V A+AV}^\pm(\mu)$, with the corresponding bare operators given by

$$\begin{aligned} \mathcal{O}_{V A+AV}^\pm &= \frac{1}{2} \left[(\bar{s}\gamma_\mu u)(\bar{u}\gamma_\mu \gamma_5 d) \pm (\bar{s}\gamma_\mu d)(\bar{u}\gamma_\mu \gamma_5 u) \right] - \frac{1}{2} [u \leftrightarrow c] + \\ &+ \frac{1}{2} \left[(\bar{s}\gamma_\mu \gamma_5 u)(\bar{u}\gamma_\mu d) \pm (\bar{s}\gamma_\mu \gamma_5 d)(\bar{u}\gamma_\mu u) \right] - \frac{1}{2} [u \leftrightarrow c]. \end{aligned} \quad (4.6)$$

4.2 Correlation functions and valence quarks

Information about the four matrix elements appearing in eqs. (4.4) and (4.5) can be extracted from suitable spatial Fourier transforms¹⁵ of the correlators ($x_0 > 0$, $z_0 > 0$ and $y_0 < 0$)

$$C_{\pm, K^0 \pi^+\pi^-}^{(\text{qcd4})}(x, z, y) = \langle \Phi_{\pi^+}(x) \Phi_{\pi^-}(z) \mathcal{O}_{V A+AV}^\pm(0) \Phi_{K^0}^\dagger(y) \rangle_{\text{conn}}, \quad (4.7)$$

$$C_{\pm, K^0 \pi^0\pi^0}^{(\text{qcd4})}(x, z, y) = \langle \Phi_{\pi^0}(x) \Phi_{\pi^0}(z) \mathcal{O}_{V A+AV}^\pm(0) \Phi_{K^0}^\dagger(y) \rangle_{\text{conn}}, \quad (4.8)$$

¹⁴As usual, the top quark contribution, which is down by a factor $O(V_{td}V_{ts}^*/V_{ud}V_{us}^* \simeq 10^{-3})$, is neglected.

¹⁵To get the kaon and the two-pion states at zero (total) three-momentum one has to sum the correlators (4.7)–(4.8) over \mathbf{y} and $(\mathbf{x} + \mathbf{z})/2$. In this way the two-pion states can be labeled by the relative three-momentum of the two pions.

where with the notation $\langle O \rangle_{\text{conn}}$ we denote the connected part of the vacuum expectation value of the multi-local operator O . As before, the superscript (qcd4) is to remind us that correlators are understood to be evaluated in the formal continuum QCD with four quark flavours (u, d, s and c). $\Phi_{K^0}, \Phi_{\pi^+}, \Phi_{\pi^-}$ and Φ_{π^0} are the interpolating operators for kaon and pion states, respectively.

Our approach here is very similar in spirit to that we have proposed in section 3 for the evaluation of B_K . In order to explain the idea it is convenient to first consider at a formal level a gauge model with, as usual, four sea quark flavours ($u_{\text{sea}}, d_{\text{sea}}, s_{\text{sea}}$ and c_{sea}), plus several (actually ten) valence quark species. For reasons that will become clear in the following, each of the up and charm valence quark species will have to be replicated four times. The pattern of valence quarks we wish to consider is then $[u, u', u'', u''', d, s, c, c', c'', c''']$. Each quark species is introduced together with the ghost necessary to cancel the loop contribution coming from the corresponding fermionic functional integration. We will denote the correlators of this model by the superscript (4s10v). We now consider the (connected) correlators

$$C_{\pm, K^0 \pi^+ \pi^-}^{(4s10v)}(x, z, y) = \langle \Phi_{\pi^+}(x) \Phi_{\pi^-}(z) \mathcal{Q}_{VA+AV}^{\pm}(0) \Phi_{K^0}^{\dagger}(y) \rangle_{\text{conn}}, \quad (4.9)$$

$$C_{\pm, K^0 \pi^0 \pi^0}^{(4s10v)}(x, z, y) = \langle \Phi_{\pi^0}(x) \Phi_{\pi^0}(z) \mathcal{Q}_{VA+AV}^{\pm}(0) \Phi_{K^0}^{\dagger}(y) \rangle_{\text{conn}}, \quad (4.10)$$

where the meson interpolating operators $\Phi_{K^0}, \Phi_{\pi^+}, \Phi_{\pi^-}$ and Φ_{π^0} are made out of the valence quarks u, d and s (but not u', u'' or u'''). This fact will be crucial for the validity of the relations (4.14)–(4.15) below. The key point in eqs. (4.9)–(4.10) is the introduction of the auxiliary operators $\mathcal{Q}_{VA+AV}^{\pm}$, defined by the formula

$$\mathcal{Q}_{VA+AV}^{\pm} = \mathcal{Q}_{VA+AV}^{\pm[0]} + \mathcal{Q}_{VA+AV}^{\pm[1]} - \frac{1}{2} \mathcal{Q}_{VA+AV}^{\pm[2]} - \frac{1}{2} \mathcal{Q}_{VA+AV}^{\pm[3]}. \quad (4.11)$$

where the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$, $k = 0, 1, 2, 3$ are all of the form (4.6), but differ from each other by the type of u and c valence quark species they contain. Explicitly we have

$$\begin{aligned} \mathcal{Q}_{VA+AV}^{\pm[k]} = & \frac{1}{2} \left[(\bar{s} \gamma_{\mu} u^{[k]}) (\bar{u}^{[k]} \gamma_{\mu} \gamma_5 d) \pm (\bar{s} \gamma_{\mu} d) (\bar{u}^{[k]} \gamma_{\mu} \gamma_5 u^{[k]}) \right] - \frac{1}{2} \left[u^{[k]} \leftrightarrow c^{[k]} \right] + \\ & + \frac{1}{2} \left[(\bar{s} \gamma_{\mu} \gamma_5 u^{[k]}) (\bar{u}^{[k]} \gamma_{\mu} d) \pm (\bar{s} \gamma_{\mu} \gamma_5 d) (\bar{u}^{[k]} \gamma_{\mu} u^{[k]}) \right] - \frac{1}{2} \left[u^{[k]} \leftrightarrow c^{[k]} \right] \end{aligned} \quad (4.12)$$

with

$$\begin{aligned} u^{[0]} &\equiv u, & u^{[1]} &\equiv u', & u^{[2]} &\equiv u'', & u^{[3]} &\equiv u''', \\ c^{[0]} &\equiv c, & c^{[1]} &\equiv c', & c^{[2]} &\equiv c'', & c^{[3]} &\equiv c'''. \end{aligned} \quad (4.13)$$

As argued in the previous section, if the two models (4s10v) and (qcd4) are regularized in the same way (say, using GW fermions), a straightforward application of the Wick theorem leads to the equalities

$$C_{\pm, K^0 \pi^+ \pi^-}^{(4s10v)}(x, z, y) = C_{\pm, K^0 \pi^+ \pi^-}^{(\text{qcd4})}(x, z, y), \quad (4.14)$$

$$C_{\pm, K^0 \pi^0 \pi^0}^{(4s10v)}(x, z, y) = C_{\pm, K^0 \pi^0 \pi^0}^{(\text{qcd4})}(x, z, y), \quad (4.15)$$

valid at any finite value of the lattice spacing, provided bare (and thus also renormalized) masses of quarks having the same flavour are given the same value in the two theories. Eqs. (4.14)–(4.15) in particular imply that the renormalization constants of the operator \mathcal{Q}_{VA+AV}^\pm in $(4s10v)$ can be taken equal to that of the operator \mathcal{O}_{VA+AV}^\pm in (qcd4) . An analogous result is obtained also for the renormalization constants of the meson interpolating operators in the two models. Under these renormalization conditions, the equalities (4.14)–(4.15) hold for the corresponding renormalized correlators and carry over to the continuum limit.

We conclude this section by offering an intuitive explanation of why we have introduced four copies of the u and c valence quarks to get all the mixings canceled. The reason is the following. For the purpose of killing the operator mixing coming from “penguin-like diagrams” it would have been enough to add to the primary u and c quarks only one extra replica of each of them, u' and c' , with $r_{u'} = -r_u$ and $r_{c'} = -r_c$ (see also section 4.5.1 below). The whole pattern is then duplicated in order to have on each gauge background the penguin-like and the non-penguin-like contractions with the correct relative multiplicity factor.

4.3 A convenient lattice discretization of the $C_{\pm, K\pi\pi}^{(4s10v)}$ correlators

In view of the previous considerations a convenient regularization of the $(4s10v)$ model is obtained by taking the action (2.1) with valence quarks $q_u \equiv u$, $q_{u'} \equiv u'$, $q_{u''} \equiv u''$, $q_{u'''} \equiv u'''$, $q_d \equiv d$, $q_s \equiv s$, $q_c \equiv c$, $q_{c'} \equiv c'$, $q_{c''} \equiv c''$ and $q_{c'''} \equiv c'''$, each having an action of the form (1.1) (accompanied by the corresponding ghosts, $\phi_u, \phi_{u'}, \dots, \phi_d, \phi_s, \phi_c, \phi_{c'}, \dots$), plus, as always, the two usual sea quark doublets, $\psi_\ell \equiv (u_{\text{sea}}, d_{\text{sea}})$ and $\psi_h \equiv (s_{\text{sea}}, c_{\text{sea}})$. For reasons which have to do with the need of making as simple as possible the renormalization pattern of the operators \mathcal{Q}_{VA+AV}^\pm , we take the Wilson parameters of the valence fields related as follows

$$\begin{aligned} r_d &= r_s, \\ r_u &= -r_{u'} = r_{u''} = -r_{u'''} = r_c = -r_{c'} = r_{c''} = -r_{c'''} . \end{aligned} \quad (4.16)$$

For definiteness, we also fix the relation between the two sets of Wilson parameters in eq. (4.16) by setting

$$r_u = r_d . \quad (4.17)$$

The choice $r_u = -r_d$ is also possible. We comment in appendix B on the implications of this (isospin breaking) choice.

The euclidean lattice theory we have just described (see also section 2) will be referred to in the following as the $(4s10v)_{tm}^L$ model.

In order for the correlators of the $(4s10v)_{tm}^L$ model (with no insertion of sea or ghost fields) to be equal to those of (qcd4) , we must require the renormalized masses of sea and valence fields to be matched as follows

$$\hat{m}_\ell^- = \hat{m}_u = \hat{m}_{u'} = \hat{m}_{u''} = \hat{m}_{u'''} , \quad \hat{m}_\ell^+ = \hat{m}_d , \quad (4.18)$$

$$\hat{m}_h^+ = \hat{m}_c = \hat{m}_{c'} = \hat{m}_{c''} = \hat{m}_{c'''} , \quad \hat{m}_h^- = \hat{m}_s . \quad (4.19)$$

Owing to eqs. (2.6)–(2.7) and the equality in absolute value of all the valence quark r parameters (eq. (4.16)), the formulae (4.18)–(4.19) fix the non-trivial relations between the bare mass parameters of sea and valence quarks and imply the bare masses of valence quarks of the same flavour to be equal, i.e.

$$m_{u'''} = m_{u''} = m_{u'} = m_u, \quad m_{c'''} = m_{c''} = m_{c'} = m_c. \quad (4.20)$$

As for the interpolating meson fields, one can use the standard pseudo-scalar quark bilinears (see, however, appendix B)

$$\Phi_{K^0}^\dagger = -\bar{d}\gamma_5 s, \quad \Phi_{\pi^+} = -\bar{d}\gamma_5 u, \quad \Phi_{\pi^-} = \Phi_{\pi^+}^\dagger = \bar{u}\gamma_5 d, \quad (4.21)$$

$$\Phi_{\pi^0} = -\Phi_{\pi^0}^\dagger = \frac{1}{\sqrt{2}} [\bar{u}\gamma_5 u - \bar{d}\gamma_5 d]. \quad (4.22)$$

The fundamental reason for considering the $(4s10v)_{tm}^L$ model with its somewhat weird valence quark content is that under the conditions (4.16) and (4.20) the $\Delta S = 1$ operators \mathcal{Q}_{VA+AV}^\pm of eq. (4.11) mix neither between themselves nor with any operator of wrong chirality or parity. This result will be proved in section 4.5 below by exploiting the symmetries of the $(4s10v)_{tm}^L$ model. As for the mixing with the famous three-dimensional operator $\bar{s}\gamma_5 d$, we will show that, just like in the formal chirally invariant continuum theory, it enters with a factor $(m_c^2 - m_u^2)(m_s - m_d)$, leaving no room for any power divergent behaviour. Similarly, despite the breaking of parity at non-zero lattice spacing, no mixing with the scalar density operator $\bar{s}d$ occurs.

It should also be recalled that in evaluating zero momentum transfer matrix elements of $\hat{\mathcal{Q}}_{VA+AV}^\pm$ (like $K \rightarrow \pi\pi$), the operator $\bar{s}\gamma_5 d$ does not play any role, because PCAC allows to write $\bar{s}\gamma_5 d = \partial_\mu(\bar{s}\gamma_\mu\gamma_5 d)/(m_s + m_d)$ from which we see that, up to contact terms, $\bar{s}\gamma_5 d$ can always be replaced by a total divergence.

At this point we can conclude that, after subtraction of the logarithmic divergent mixing of \mathcal{Q}_{VA+AV}^\pm with $(m_c^2 - m_u^2)(m_s - m_d)\bar{s}\gamma_5 d$ (whenever needed), and multiplication by the appropriate renormalization constants, the correlators (4.9) and (4.10), evaluated in the $(4s10v)_{tm}^L$ model, admit a well defined continuum limit. The limiting quantities, under the conditions (4.18)–(4.19), coincide with the (continuum limit of the) correlators (4.7)–(4.8) in the (qcd4) model, thanks to the equalities (4.14)–(4.15).

4.4 Some observations

A number of observations are in order at this point. First of all, we stress that, on the basis of the general arguments given in section 2, the correlators (4.9)–(4.10) can be $\mathcal{O}(a)$ improved via WA 's (see eq. (2.22)). Actually, owing to the symmetry under $\mathcal{P} \times (R \rightarrow -R)$ enjoyed by the $(4s10v)_{tm}^L$ model, the necessary WA 's of the matrix elements of interest can be constructed in terms of data obtained from a single simulation, as explained in section 2.3.2, by averaging — whenever necessary — matrix elements with opposite value of the relative three-momentum of the two pions.

Secondly, for completeness we recall that, in order to actually extract from simulation data the amplitudes $\mathcal{A}_{K^0 \rightarrow \pi^+ \pi^-}$ and $\mathcal{A}_{K^0 \rightarrow \pi^0 \pi^0}$, it is also necessary to evaluate some extra

two- and four-point correlation functions, such as

$$\begin{aligned} &\langle \Phi_{K^0}(x) \Phi_{K^0}^\dagger(x') \rangle, \quad \langle \Phi_{\pi^+}(x) \Phi_{\pi^+}^\dagger(x') \rangle, \quad \langle \Phi_{\pi^0}(x) \Phi_{\pi^0}(x') \rangle_{\text{conn}}, \\ &\langle \Phi_{\pi^+}(x) \Phi_{\pi^+}^\dagger(z) \Phi_{\pi^+}(x') \Phi_{\pi^+}^\dagger(z') \rangle_{\text{conn}}, \quad \langle \Phi_{\pi^0}(x) \Phi_{\pi^0}(z) \Phi_{\pi^0}(x') \Phi_{\pi^0}(z') \rangle_{\text{conn}}, \end{aligned} \quad (4.23)$$

where in the last two four-point correlators one should take $x_0, z_0 > 0$ and $x'_0, z'_0 < 0$. Suitable spatial Fourier transforms of these correlators provide the necessary extra information on the energies of the kaon, single pion and two-pion states, as well as on the $\pi\pi$ -phase shift [23, 24], which will in principle enable us to extract the physical decay amplitudes of interest. Finally, when not automatic, the correlators (4.23) can be $\mathcal{O}(a)$ improved by taking appropriate WA 's.

Once the bare amplitudes of interest have been evaluated with no $\mathcal{O}(a)$ cut-off effects, a non-perturbative lattice estimate of the renormalization constants, $Z_{VA+AV}^\pm(a\mu)$, is required. The latter can be obtained following the strategy outlined in section 3.3 of ref. [2]. One could e.g. consider a correlator where \mathcal{Q}_{VA+AV}^\pm is inserted at zero three-momentum with some other local m.r. operator having appropriate quantum numbers so as not to get an identically vanishing two-point function (see also section 2.3.2).

In the same spirit of the observation made at the end of section 3.2, we note that one can eliminate the flavour species u''' and c''' from the game (as they are indistinguishable from u' and c' , respectively) and change the form of the operator in eq. (4.11) with the substitution

$$\mathcal{Q}_{VA+AV}^\pm \rightarrow \mathcal{Q}_{VA+AV}^{\pm[0]} + \frac{1}{2} \mathcal{Q}_{VA+AV}^{\pm[1]} - \frac{1}{2} \mathcal{Q}_{VA+AV}^{\pm[2]}. \quad (4.24)$$

Again, in this framework the proof of absence of mixing becomes somewhat more complicated than the one we give below.

4.5 The renormalization properties of \mathcal{Q}_{VA+AV}^\pm

In this section we want to prove that the operators \mathcal{Q}_{VA+AV}^\pm (eq. (4.11)) do not mix with any operator of lower or equal dimension, having either wrong chirality or opposite parity, precisely as in the formal continuum theory or within chirally invariant lattice regularizations (like those provided by fermions obeying the GW condition). This in practice means that no mixing with operators of the same or lower dimension is relevant for the computation of the $K \rightarrow \pi\pi$ decay amplitudes. In the arguments of this section a crucial role is played by the conditions (4.16) and (4.20), which are always assumed as part of the specification of the lattice $(4s10v)_{tm}^L$ model we consider. Thanks to eq. (4.16) and the condition $|r_u| = |r_d|$, the valence flavour symmetries of the action (2.1) rule out the mixing of \mathcal{Q}_{VA+AV}^+ and \mathcal{Q}_{VA+AV}^- between themselves (see appendix C for details), as in the case of untwisted Wilson fermions. We can hence deal “in parallel” with \mathcal{Q}_{VA+AV}^+ and \mathcal{Q}_{VA+AV}^- .

4.5.1 Operators of dimension lower than six

Gauge, $H(4)$ and \mathcal{I}_f (with $f = s, d$, see eq. (2.9)) invariances of the $(4s10v)_{tm}^L$ lattice model restrict the possible operators of dimension less than six which \mathcal{Q}_{VA+AV}^\pm can mix with to

only the following ones

$$\bar{s}\gamma_5 d, \quad \bar{s}d, \quad \bar{s}\gamma_5\sigma\cdot Fd, \quad \bar{s}\sigma\cdot Fd, \quad (4.25)$$

where $\sigma\cdot F = \sigma_{\mu\nu}F_{\mu\nu}[U]$ and $F_{\mu\nu}[U]$ stands for any lattice discretization of the gluon field strength.

We wish to show now that, thanks to the (spurionic) symmetries enjoyed by the $(4s10v)_{tm}^L$ lattice model, the above operators can only come into play multiplied by at least three powers of quark masses, according to the pattern given below

$$(m_c - m_u)(m_c + m_u)(m_s - m_d) \quad \bar{s}\gamma_5 d, \quad (4.26)$$

$$(m_c - m_u)(m_c + m_u)(m_s - m_d)(m_s + m_d) \quad \bar{s}d, \quad (4.27)$$

$$(m_c - m_u)(m_c + m_u)(m_s - m_d) \quad \bar{s}\gamma_5\sigma\cdot Fd, \quad (4.28)$$

$$(m_c - m_u)(m_c + m_u)(m_s - m_d)(m_s + m_d) \quad \bar{s}\sigma\cdot Fd. \quad (4.29)$$

As a result, for obvious dimensional reasons none of the above operators can appear multiplied by power divergent mixing coefficients. Only the operator (4.26) will enter with a logarithmically divergent coefficient. However, as we have already discussed in section 4.3, it gives vanishing contributions to the physical decay amplitudes. One might add that the mass factor in front of it vanishes anyway in the chiral limit or in the limit of exact $SU_V(3)$.

Since the operators $\bar{s}\gamma_5 d$ and $\bar{s}\gamma_5\sigma\cdot Fd$ (as well as $\bar{s}d$ and $\bar{s}\sigma\cdot Fd$) have identical transformation properties under all the symmetries we will be using in the argument that follows, it is sufficient to restrict our attention to the operators (4.26) and (4.27). Consistently with this observation we notice that the overall quark mass factor in front of the operators (4.28) and (4.29) is the same as that appearing in front of the operators (4.26) and (4.27), respectively.

We give a proof of the structure of the mass dependence displayed in eqs. (4.26) and (4.27) in four steps.

1. The presence of the factor $(m_c - m_u)$ follows from the spurionic invariance of the lattice action (2.1) of the $(4s10v)_{tm}^L$ model under the transformation

$$\text{Ex}(u, c) \times \text{Ex}(u', c') \times \text{Ex}(u'', c'') \times \text{Ex}(u''', c''') \times (m_u \leftrightarrow m_c), \quad (4.30)$$

where $\text{Ex}(f_1, f_2)$ is defined in eq. (3.16). Indeed, under (4.30) the operators \mathcal{Q}_{VA+AV}^\pm are odd, while $\bar{s}\gamma_5 d$ and $\bar{s}d$ are both even, as they are left untouched by the transformation.

2. The presence of the factor $(m_s - m_d)$, is a consequence of the spurionic invariance of the action under the transformation

$$\text{Ex}(d, s) \times \mathcal{C} \times (m_d \leftrightarrow m_s), \quad (4.31)$$

where \mathcal{C} is the charge conjugation operation (eq. (A.1)). Under the transformation (4.31) the operators \mathcal{Q}_{VA+AV}^\pm are odd, while $\bar{s}\gamma_5 d$ and $\bar{s}d$ are even.

3. At this stage we have proven that both the operators $\bar{s}\gamma_5 d$ and $\bar{s}d$ must appear multiplied by a factor of the form $(m_c - m_u)(m_s - m_d)$. Based on this result we now show that a further factor $(m_c + m_u)$ must be present owing to the spurionic invariance of the action under the transformation

$$\begin{aligned} & \text{Ex}_5(u, u') \times \text{Ex}_5(u'', u''') \times (m_u \rightarrow -m_u) \times \\ & \times \text{Ex}_5(c, c') \times \text{Ex}_5(c'', c''') \times (m_c \rightarrow -m_c), \end{aligned} \quad (4.32)$$

where $\text{Ex}_5(f_1, f_2)$ is defined in eq. (3.17). In fact, under the transformation (4.32) the operators \mathcal{Q}_{VA+AV}^\pm are even, while the combinations $(m_c - m_u)\bar{s}\gamma_5 d$ and $(m_c - m_u)\bar{s}d$ are odd. Consequently, the mass factor in front of both operators will have to have the form $(m_c^2 - m_u^2)(m_s - m_d)$. Thus the GIM suppression factor turns out to be quadratic just like in the continuum.

We remark that each of the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$, $k = 0, 1, 2, 3$, that make up \mathcal{Q}_{VA+AV}^\pm , actually mixes with $(m_c - m_u)(m_s - m_d)\bar{s}\gamma_5 d$ and $(m_c - m_u)(m_s - m_d)\bar{s}d$, with linearly divergent coefficients. Owing to the spurionic invariance $\mathcal{R}_{5u[k]}^{\text{sp}} \times \mathcal{R}_{5c[k]}^{\text{sp}}$ (eq. (2.16)), such coefficients are, however, odd in $r_{u[k]} = r_{c[k]}$. As a consequence of this property and the peculiar valence flavour structure of the regularization we have introduced (see eq. (4.16)), all the mixings with lower dimensional operators cancel against each other in the combination (4.11), which is symmetric under $(u, c) \leftrightarrow (u', c')$ and $(u'', c'') \leftrightarrow (u''', c''')$.

4. On the basis of the further spurionic invariance of the lattice action under the transformation

$$\mathcal{P}_5 \times (M \rightarrow -M), \quad (4.33)$$

where \mathcal{P}_5 is defined in eq. (A.9), one concludes that the mixing of \mathcal{Q}_{VA+AV}^\pm with $\bar{s}d$ must be suppressed by an extra quark mass factor, besides $(m_c^2 - m_u^2)$ and $(m_s - m_d)$. This is so because the operators \mathcal{Q}_{VA+AV}^\pm are odd under the transformation (4.33), precisely as $(m_c^2 - m_u^2)(m_s - m_d)\bar{s}\gamma_5 d$, while the combination $(m_c^2 - m_u^2)(m_s - m_d)\bar{s}d$ is even. In front of the latter a further mass factor must hence be present, which for consistency with the symmetries (4.30), (4.31) and (4.32) can only be of the form $(m_s + m_d)$. We get in this way the expression anticipated in eq. (4.27), which we notice is a mere $\mathcal{O}(a)$ cut-off effect. Its contribution actually cancels in Wilson-averaged correlators and derived matrix elements.

We have thus proved that the operators \mathcal{Q}_{VA+AV}^\pm do not mix with operators of dimension lower than six.

4.5.2 Operators of dimension six

The operators \mathcal{Q}_{VA+AV}^\pm (eq. (4.11)) are linear combinations of the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$, defined in eq. (4.12). The latter — according to the notation introduced in (4.13) — contain, besides the valence d and s quarks, the flavour species u and c when $k = 0$, u' and c' when $k = 1$, u'' and c'' when $k = 2$ and finally u''' and c''' when $k = 3$.

The somewhat involved proof that the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$, $k \in \{0, 1, 2, 3\}$ and, hence, $\mathcal{Q}_{VA+AV}^{\pm}$ (eq. (4.11)) mix neither between themselves nor with any other operator of dimension six is given in appendix C.¹⁶

Incidentally we remark that the overall renormalization constant of each $\mathcal{Q}_{VA+AV}^{\pm[k]}$ does not depend on the sign of $r_{u[k]} = r_{c[k]}$ (see eq. (4.16)), owing to the general argument given below eq. (2.21). Since all the valence Wilson parameters are taken to be equal in absolute value, it follows that the renormalization constant of $\mathcal{Q}_{VA+AV}^{\pm[k]}$ is actually independent of k , i.e. is the same for all the terms that make up $\mathcal{Q}_{VA+AV}^{\pm}$.

5. The $\Delta I = 1/2$ rule from $K \rightarrow \pi$ amplitudes

In the chiral limit $K \rightarrow \pi\pi$ amplitudes can be related to $K \rightarrow \pi$ and $K \rightarrow \text{vacuum}$ amplitudes by the soft pion theorems (SPT's) [33] of Current Algebra [34]. The interest of these formulae lies in the fact that they allow to evaluate in the chiral limit $K \rightarrow \pi\pi$ amplitudes from the knowledge of $K \rightarrow \pi$ matrix elements which are simpler to compute numerically because the final (and the initial) state is a one-particle state and the no-go theorem of ref. [22] does not apply. Naturally, as these relations are among amplitudes evaluated in the limit of vanishing quark masses, a non-trivial extrapolation to the physical mass point will have to be performed.

Starting again from eq. (4.2), it can be proved [19, 31, 32, 13] that in QCD with four flavours it is enough to compute (for a range of quark masses and momenta of the kaon and pion states) the matrix elements

$$\langle \pi^+(p) | \hat{\mathcal{O}}_{VV+AA}^{\pm} | K^+(q) \rangle, \quad \langle \pi^0(p) | \hat{\mathcal{O}}_{VV+AA}^{\pm} | K^0(q) \rangle, \quad (5.1)$$

where the bare expression of the parity even operators $\hat{\mathcal{O}}_{VV+AA}^{\pm}$ reads

$$\begin{aligned} \mathcal{O}_{VV+AA}^{\pm} = & \frac{1}{2} \left[(\bar{s}\gamma_{\mu}u)(\bar{u}\gamma_{\mu}d) \pm (\bar{s}\gamma_{\mu}d)(\bar{u}\gamma_{\mu}u) \right] - \frac{1}{2} [u \leftrightarrow c] + \\ & + \frac{1}{2} \left[(\bar{s}\gamma_{\mu}\gamma_5u)(\bar{u}\gamma_{\mu}\gamma_5d) \pm (\bar{s}\gamma_{\mu}\gamma_5d)(\bar{u}\gamma_{\mu}\gamma_5u) \right] - \frac{1}{2} [u \leftrightarrow c]. \end{aligned} \quad (5.2)$$

Following a strategy analogous to the one developed in the previous section, we want to prove that the matrix elements (5.1) can be extracted (actually with no $\mathcal{O}(a)$ cut-off effects) from correlation functions defined in an auxiliary lattice regularized theory where the relevant four fermion operators do not mix with any other operator of wrong chirality or opposite parity.

5.1 Correlation functions and valence quarks

Let us start by noting that the four matrix elements appearing in eq. (5.1) can be obtained in the formal continuum QCD theory with four quark flavours (qcd4) from (suitable Fourier transforms of) the correlators

$$C_{\pm, K\pi}^{(\text{qcd4})}(x, y) = \langle \Phi_{\pi}(x) \mathcal{O}_{VV+AA}^{\pm}(0) \Phi_K^{\dagger}(y) \rangle_{\text{conn}} \quad (5.3)$$

with K and π being either K^0 and π^0 or K^+ and π^+ .

¹⁶As we have already pointed out, the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$ separately do mix with operators of lower dimensions. But in the relevant combination of eq. (4.11) the latter cancel out and arrange themselves so as to give rise precisely to the pattern of eqs. (4.26) to (4.29), as was shown in section 4.5.1.

Always at a formal level, we need to consider again the $(4s10v)$ model that was introduced in section 4.2. We are interested now in the correlators

$$C_{\pm, K\pi}^{(4s10v)}(x, y) = \langle \Phi_\pi(x) \mathcal{Q}_{VV+AA}^\pm(0) \Phi_K^\dagger(y) \rangle_{\text{conn}}, \quad (5.4)$$

where the meson interpolating operators Φ_K and Φ_π are made out exclusively of the valence quarks u , d and s , while the operators \mathcal{Q}_{VV+AA}^\pm are given by

$$\mathcal{Q}_{VV+AA}^\pm = \mathcal{Q}_{VV+AA}^{\pm[0]} + \mathcal{Q}_{VV+AA}^{\pm[1]} - \frac{1}{2} \mathcal{Q}_{VV+AA}^{\pm[2]} - \frac{1}{2} \mathcal{Q}_{VV+AA}^{\pm[3]}, \quad (5.5)$$

$$\begin{aligned} \mathcal{Q}_{VV+AA}^{\pm[k]} = & \frac{1}{2} \left[(\bar{s} \gamma_\mu u^{[k]}) (\bar{u}^{[k]} \gamma_\mu d) \pm (\bar{s} \gamma_\mu d) (\bar{u}^{[k]} \gamma_\mu u^{[k]}) \right] - \frac{1}{2} \left[u^{[k]} \leftrightarrow c^{[k]} \right] + \\ & + \frac{1}{2} \left[(\bar{s} \gamma_\mu \gamma_5 u^{[k]}) (\bar{u}^{[k]} \gamma_\mu \gamma_5 d) \pm (\bar{s} \gamma_\mu \gamma_5 d) (\bar{u}^{[k]} \gamma_\mu \gamma_5 u^{[k]}) \right] - \frac{1}{2} \left[u^{[k]} \leftrightarrow c^{[k]} \right]. \end{aligned} \quad (5.6)$$

As in the previous section, if the two $(4s10v)$ and (qcd4) models are regularized in the same way (say, using GW fermions), a straightforward application of Wick theorem leads to the equalities

$$C_{\pm, K\pi}^{(4s10v)}(x, y) = C_{\pm, K\pi}^{(\text{qcd4})}(x, y), \quad (5.7)$$

valid at any finite value of the lattice spacing, provided bare (and thus also renormalized) quark masses of the same flavour are given identical numerical values in the two theories. Eqs. (5.7) in particular imply that the renormalization constants of the operators \mathcal{Q}_{VV+AA}^\pm in $(4s10v)$ can be taken equal to those of the operators \mathcal{O}_{VV+AA}^\pm in (qcd4) . The same equality holds for the kaon and pion interpolating fields. With this natural choice of renormalization conditions eqs. (5.7) are valid for the corresponding renormalized correlators and carry over to the continuum limit.

5.2 A convenient lattice discretization of the $C_{\pm, K\pi}^{(4s10v)}$ correlators

For the purpose of getting rid of all mixing problems in the process of computing the matrix elements (5.1), we will have to regularize the $(4s10v)$ model in way which is slightly different from that we followed in section 4.3. Namely, we now have to take

$$\begin{aligned} -r_s &= r_d, \\ r_u &= -r_{u'} = r_{u''} = -r_{u'''} = r_c = -r_{c'} = r_{c''} = -r_{c'''} \end{aligned} \quad (5.8)$$

and fix the relation between the two sets of Wilson parameters in eq. (5.8) by setting¹⁷

$$r_u = r_d. \quad (5.9)$$

This lattice regularized model will be denoted in the following as $(4s10v)_{tm}^{L*}$. We stress that it differs from the lattice model $(4s10v)_{tm}^L$ of section 4.3 only by the sign of r_s relative to $r_d = r_u$ (and to all the remaining valence Wilson parameters). Naturally, in order to obtain

¹⁷This choice is made for convenience, i.e. to directly exploit the results of the previous section in the argument we will give in section 5.3 and also to have, for $m_d = m_u$, exact isospin symmetry in the u and d valence quark sector. However, for the purpose of canceling unwanted mixings only the condition $|r_u| = |r_d|$ is necessary (see appendix B).

from the $(4s10v)_{tm}^{L*}$ model correlators that in the continuum limit are equivalent to those of (qcd4), the quark mass renormalization conditions (4.18)–(4.19) have to be imposed. As in section 3.1 such conditions entail eq. (4.20).

In practice to extract the matrix elements (5.1), besides the three-point correlators (5.4), it will be necessary to evaluate in the $(4s10v)_{tm}^{L*}$ model also two-point correlators of the type

$$\langle \Phi_\pi(x) \Phi_\pi^\dagger(x') \rangle_{\text{conn}}, \quad \langle \Phi_K(x) \Phi_K^\dagger(x') \rangle. \quad (5.10)$$

Suitable spatial Fourier transforms of these two- and three-point correlation functions contain all the information which is necessary in order to extract the desired $K \rightarrow \pi$ matrix element. The correlators (5.4) and (5.10) can be $O(a)$ improved by taking appropriate WA 's or by averaging over amplitudes computed with opposite signs of the K and π three-momenta.

Analogously to the $K \rightarrow \pi\pi$ case previously discussed, also here one could eliminate the valence quark species u''' and c''' and accordingly modify the expression of the operator (5.5) with the substitution

$$\mathcal{Q}_{VV+AA}^\pm \rightarrow \mathcal{Q}_{VV+AA}^{\pm[0]} + \frac{1}{2} \mathcal{Q}_{VAV+AA}^{\pm[1]} - \frac{1}{2} \mathcal{Q}_{VV+AA}^{\pm[2]}. \quad (5.11)$$

5.3 The renormalization properties of \mathcal{Q}_{VV+AA}^\pm

Proving that in the $(4s10v)_{tm}^{L*}$ model the operator \mathcal{Q}_{VV+AA}^\pm (eq. (5.5)) does not mix with any other operator is immediate from the results of section 4.5. It suffices, in fact, to perform in the functional integrals that defines the relevant correlation functions of the $(4s10v)_{tm}^{L*}$ model the change of fermionic integration variables induced by the transformation \mathcal{R}_{5s} (see eq. (2.10)). The reason is that under this transformation 1) the action of the $(4s10v)_{tm}^{L*}$ model turns into that of the $(4s10v)_{tm}^L$ model except for a sign inversion in front of the s quark mass term; 2) the operator \mathcal{Q}_{VV+AA}^\pm is transformed into the operator \mathcal{Q}_{VA+AV}^\pm . At this point we are exactly in the situation we have discussed in section 4, except that we have to carry out the transformation \mathcal{R}_{5s} on the list of operators (4.26) to (4.29) and invert the sign of m_s in all formulae we previously got. Thus, the pattern of eqs. (4.26) to (4.29) gets modified as follows

$$(m_c - m_u)(m_c + m_u)(m_s + m_d) \quad \bar{s}d, \quad (5.12)$$

$$(m_c - m_u)(m_c + m_u)(m_s + m_d)(m_s - m_d) \quad \bar{s}\gamma_5 d, \quad (5.13)$$

$$(m_c - m_u)(m_c + m_u)(m_s + m_d) \quad \bar{s}\sigma \cdot F d, \quad (5.14)$$

$$(m_c - m_u)(m_c + m_u)(m_s + m_d)(m_s - m_d) \quad \bar{s}\sigma \cdot F \gamma_5 d. \quad (5.15)$$

The mass factors appearing in eqs. (5.13) and (5.15) in front of the operators $\bar{s}\gamma_5 d$ and $\bar{s}\gamma_5 \sigma \cdot F d$ depend quadratically on m_s , so they are left unchanged. Furthermore, the whole line of arguments we gave before to prove that \mathcal{Q}_{VA+AV}^\pm could not mix with operators of dimension six in the $(4s10v)_{tm}^L$ model can be applied to infer the same property for the operators \mathcal{Q}_{VV+AA}^\pm in the $(4s10v)_{tm}^{L*}$ model, as dimensionless mixing coefficients are independent of the quark mass (in a mass independent renormalization scheme). This concludes our proof.

The net result of this analysis is that the situation is just like in continuum massive QCD. Only the particular combination appearing in eq. (5.12) needs a (logarithmically) divergent coefficient, were this subtraction required. This term, however, will not contribute to the $K \rightarrow \pi$ form factor that is related through SPT's to the $K \rightarrow \pi\pi$ amplitude, because SPT's have to be understood as relations between amplitudes evaluated in the chiral limit.

Concerning the renormalization constants of the operators \mathcal{Q}_{VV+AA}^\pm in the model $(4s10v)_{tm}^*$, it is clear that they are equal to those of the operators \mathcal{Q}_{VA+AV}^\pm in the model $(4s10v)_{tm}^L$ (see comments on the evaluation of Z_{VA+AV}^\pm at the end of section 4.3). The reason is simply that, as pointed out before, the change of fermionic integration variables induced by the transformation \mathcal{R}_{5s} exactly maps the two theories and the two operators one into the other.

6. Concluding remarks

Our present knowledge of QCD offers a deep understanding of strong interaction physics with two noticeable exceptions. One is the lack of a convincing solution of the strong-CP problem [35], the second is the difficulty of finding a physically sound explanation of the anomalously large value of the $R(K \rightarrow \pi\pi)$ (eq. (4.1)).

Clarification of anyone of these two issues may have a significant impact on the structure of any forthcoming unified theory comprising the Standard Model, or give hints about possible signals of new physics already at low energy, though it is likely that the strong CP-problem cannot have a solution within QCD [36], but requires its embedding in a larger theory.¹⁸

In this perspective the results of the present paper look rather interesting, because, when put together with those of refs. [2, 4], set the basis for a workable framework, where a first principle computation of the matrix elements of the CP-conserving $\Delta S = 1$ and $\Delta S = 2$ effective weak hamiltonian at realistic values of the light quark masses appears to be feasible with the computer resources that are or will be soon available. A more precise estimate of the requested computational effort will be possible as soon as the practical issues concerning the magnitude of residual cutoff effects, in particular for light quarks, and possible lattice phase transitions in unquenched simulations (see the discussion below) will be clarified.

Independently of these practical issues, the use of maximally twisted Wilson (or rather Osterwalder-Seiler) fermions, according to the strategy advocated in this paper, brings about conceptual and qualitative progresses which can be summarized as follows:

1. no zero modes of the Wilson-Dirac operator at non-vanishing quark masses (in particular no exceptional configurations);
2. a positive definite fermionic determinant, even for mass non-degenerate quarks, in unquenched studies with an even number of dynamical flavours (in this paper we focused on the phenomenologically relevant case of four flavours);

¹⁸See, however, the papers in ref. [37] for a possible solution within QCD itself.

3. no contribution from wrong chirality or opposite parity mixing for the lattice operators entering the computation of the weak matrix elements of interest;
4. automatic (or easily obtainable) $O(a)$ improvement of all relevant physical quantities.

Although the method we propose is rather general, in this paper for definiteness it has been applied only to the (important) instance of the evaluation of the B_K parameter entering the $K^0\text{--}\bar{K}^0$ mixing and the $K \rightarrow \pi\pi$, or $K \rightarrow \pi$, amplitude. In the lattice computational framework we propose

- the B_K parameter can be hopefully computed including sea quark effects, with a sufficiently small error, so as to significantly reduce one of the largest theoretical uncertainty in the phenomenology of the unitarity triangle [15];
- the yet elusive $\Delta I = 1/2$ signal does not appear to be anymore buried underneath a numerically overwhelming, divergent subtraction (as was the case for Wilson fermions).

These results are obtained at a surprisingly low price. Sea quarks need to be introduced in pairs and a somewhat exotic pattern of valence quarks has to be used in the construction of the effective weak hamiltonian lattice operator.

From several viewpoints the situation is thus very much like with GW fermions, where chiral symmetry is exact and cut-off effects only show up at $O(a^2)$. The non-negligible gain that we get with the strategy we are advocating here is that the computational burden appears to be significantly reduced with respect to simulations involving GW fermions. This feature makes our method potentially suited for the study of systems with a physical linear size of a few fermi, while including sea quark effects. In comparison to approaches based on untwisted Wilson fermions (which are, however, plagued with complicated operator mixing and the problem of “exceptional configurations”), the method we propose possibly requires a little more extra computing time, owing to the need of computing certain valence quark propagators for opposite values of the Wilson parameter. This overhead is more than compensated at small quark masses by the expected improvement in the performance of linear solvers, due to the protection against spurious quark zero modes that is guaranteed by twisting.

6.1 Critical mass and $O(a)$ improvement

It should be noted that our work is not based on any special definition of the critical mass for sea and valence quarks (see eqs. (2.4)–(2.5)). The method for $O(a)$ improvement discussed in section 2.3, which is a straightforward generalization of the approach presented in ref. [2], relies only on the property that $f_{\text{cr}}(r_1; r_2, r_3)$ is an odd function of r_1 , implying that the sea and valence critical masses, $M_{\text{cr}}(r_{\ell,h})$ and $M_{\text{cr}}(r_f)$ are in turn odd in $r_{\ell,h}$ and r_f , respectively. The argument showing that f_{cr} is odd in r_1 we give here (in section 2.1 and appendix A) is analogous to that presented in ref. [2] in the case of generic (chirally twisted) Wilson fermions.

The question of the r -parity properties of $M_{\text{cr}}(r)$ was taken up in refs. [38, 39]. Clearly this issue could have an impact on the question of $O(a)$ improvement as we have discussed it in the present paper and in ref. [2]. Actually, it turns out that $M_{\text{cr}}(r)$ can and should always be taken odd in r .

The reason is simply that any counterterm to be included in the process of renormalizing the theory should not break any of the symmetries the classical action enjoys prior to renormalization. Indeed, the manifold of the possible solutions for M_{cr} , defined by whichever condition one wishes to take, has the property of being reflected around zero under the transformation $r \rightarrow -r$ (see e.g. ref. [40] for a discussion of this point). Thus it would be unwise and not very useful to violate the (spurionic) symmetries of the theory (in particular $\mathcal{P} \times (R \rightarrow -R)$) by having a critical mass that, for instance, to some $O(a^p)$ with $p > 1$, is not odd in r .

Apart from this observation, it is important to remark that the whole issue of $O(a)$ improvement, as it is discussed in ref. [2] and in this paper, assumes that as $a \rightarrow 0$ the counting of powers of a is done by taking the renormalized quark masses fixed. We did not address the interesting question of what happens when the quark mass is taken to be a quantity of $O(a)$ or $O(a^2)$, as often done in papers dealing with lattice chiral perturbation theory [38, 39, 41, 42, 43].

6.2 Tests and numerical issues

The numerical effectiveness of the whole approach based on maximally twisted Wilson quarks has to be carefully checked, especially for small quark masses and when taking into account the effects of sea quarks.

There are already encouraging results, coming from the quenched simulations of ref. [12] and the analytic work of ref. [41], indicating that the scaling behaviour of the theory is indeed smoother and flatter than with standard or clover-improved Wilson fermions. An extension of the scaling tests of ref. [12] to several lower values of the pseudoscalar meson mass, down to less than 300 MeV, is currently in progress [44].

Furthermore, recently, an exploratory study of the effects of unquenching in simulations of tm-LQCD with two mass degenerate quarks on rather coarse lattices of size $8^3 \times 16$, $12^3 \times 24$ and $16^3 \times 32$ at $\beta = 5.2$ (using the standard Wilson plaquette action) was presented [45]. In this work the PCAC quark mass, m_{χ}^{PCAC} (see eq. (12) of ref. [45]), the mass of the pion and the plaquette expectation value have been measured at $am_{\ell} = 0.01$,¹⁹ as functions of the untwisted mass, m_0 .²⁰

Results show features of the kind suggested by refs. [46, 42, 43] in the framework of chiral perturbation theory, when the order of magnitude inequality $a^2 \Lambda_{\text{QCD}}^2 \ll am_{\ell}$ is not satisfied [2]. Metastabilities are detected, signalled by the behaviour of the plaquette expectation value which is seen to undergo hysteresis cycles as m_0 is driven through M_{cr} . In this situation gauge configurations cannot be considered as properly thermalized. Metastable states associated with values of m_{χ}^{PCAC} of different sign have been identified and argued to

¹⁹In the notation of ref. [45] $m_{\ell} \equiv \mu$.

²⁰Introducing m_0 in the action (2.1) amounts to replacing there W_{cr} with $W_{\text{cr}} - M_{\text{cr}} + m_0$.

stem from the effective lack of criticality of the subtracted Wilson term and the associated existence of non-zero values for the parity and flavour breaking quark condensates. As a consequence, one does not yet observe the expected vanishing of m_χ^{PCAC} at a critical value of m_0 (providing a natural definition of M_{cr}). It is, however, reassuring to see that the squared pion mass appears to be roughly proportional to $\sqrt{(Z_A m_\chi^{PCAC})^2 + m_\ell^2}$ in both the observed metastable branches.

On the basis of the present understanding [43] of the metastability phenomena discussed above, we expect them to get weaker and weaker and eventually disappear as the lattice spacing is decreased, making thus possible the evaluation of physical quantities with controlled $O(a^2)$ cut-off effects. Preliminary data [47] coming from simulations in progress at $\beta = 5.3$ seem to be consistent with such an expectation.

6.3 Outlook

The idea of using a hybrid approach where valence and sea quarks are regularized in different fashion was already put forward in the literature (see, for instance, ref. [48] and references therein). Along this line a winning strategy, where all the nice properties we have listed above remain valid, could be to use GW fermions as valence quarks and maximally twisted quark pairs in loops. With this choice one could ease the problem related to the need of working at relatively large values of β (and correspondingly large lattices) if the valence quark mass is small, and obtain a computational framework, where CPU times for inverting the overlap Dirac operator and stochastically taking into account the fermion determinant are comparable.

We end by recalling that the tm-LQCD action can also be employed [1, 49] in the framework of the Schrödinger functional formalism [50]. Results about the $O(a)$ improvement remain valid for quantities that are independent of the boundary conditions, like on-shell matrix elements or masses. However, if one wishes to improve the whole Schrödinger functional, which is a necessary step in order to get cancellation of $O(a)$ cut-off effects in the evaluation of, for instance, the running gauge coupling, quark masses and renormalization constants, the way of extending the WA method is not completely obvious and will be the object of a forthcoming publication [51].

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A. Renormalizability of the lattice model (2.1)

We want to show in this appendix that the action of the lattice model (2.1) contains all the terms of dimension not larger than four, allowed by the action symmetries, that are required for correlators with no ghost fields be renormalizable. In the course of this discussion we also prove 1) the results contained in eqs. (2.6)–(2.7), 2) the property that

a unique function, $f_{\text{cr}}(r; r_\ell, r_h)$, determines the critical mass of OS valence and twisted sea quarks (see eqs. (2.4)–(2.5)) and 3) the relation $Z_m(r_f) = Z_P(r_f)^{-1}$ for $r_f = r_\ell$ or $r_f = r_h$.

We start by noticing that completely standard arguments, based on dimensionality and invariance of the action (2.1) under lattice gauge transformations, translations, $H(4)$ rotations and charge conjugation,

$$\mathcal{C} : \begin{cases} U_\mu(x) \rightarrow U_\mu^*(x) \\ \psi_p(x) \rightarrow i\gamma_0\gamma_2\bar{\psi}_p^T(x), & \bar{\psi}_p(x) \rightarrow -\psi_p^T(x)i\gamma_0\gamma_2, & p = \ell, h \\ q_f(x) \rightarrow i\gamma_0\gamma_2\bar{q}_f^T(x), & \bar{q}_f(x) \rightarrow -q_f^T(x)i\gamma_0\gamma_2, & \text{all } f'\text{'s} \\ \phi_f(x) \rightarrow i\gamma_0\gamma_2(\phi_f^\dagger)^T(x) = i\gamma_0\gamma_2\phi_f^*(x), & & \text{all } f'\text{'s} \end{cases}, \quad (\text{A.1})$$

imply that the only relevant action density terms are, besides gauge invariant gluonic operators (FF and $F\tilde{F}$), either fermionic bilinears of the type $\bar{\psi}_p \dots \psi_p$ and $\bar{q}_f \dots q_f$ or ghost bilinears of the form $\phi_f^\dagger \dots \phi_f$.

A.1 Sea quark sector

The renormalization of correlation functions with only gluons and $\psi_{\ell,h}, \bar{\psi}_{\ell,h}$ fields proceeds as discussed in ref. [4]. In fact, for this class of correlation functions the contributions coming from functionally integrating valence quark and ghost fields completely cancel against each other, while the symmetries discussed in ref. [4] are straightforwardly extended from one to two pairs of maximally twisted quarks.²¹

Furthermore mixed sea quark action terms of the form $\bar{\psi}_\ell \dots \psi_h$ or $\bar{\psi}_h \dots \psi_\ell$ can not arise, as it trivially follows from the invariance of the action under the independent $U(1)$ vector transformations

$$\mathcal{I}_p : \psi_p(x) \rightarrow e^{i\theta_p}\psi_p(x), \quad \bar{\psi}_p(x) \rightarrow \bar{\psi}_p(x)e^{-i\theta_p}, \quad p = \ell, h. \quad (\text{A.2})$$

The important equation (2.6) can be derived from the analysis of the chiral WTI's of the lattice model (2.1) involving correlators with the insertion of $\psi_{\ell,h}$ and $\bar{\psi}_{\ell,h}$ fields only. Since valence quarks are totally inert, the structure of these WTI's is identical to that reported in ref. [4] for maximally twisted lattice QCD with one pair of mass non-degenerate quarks. For the reader convenience we report here the WTI's from which the renormalization properties of the quark masses most straightforwardly follow. If $\hat{O}(y)$ is a renormalized (multi-local) operator, one gets, among others, the two WTI's ($x \neq y$)

$$\left\langle \left(\partial_\mu^* \hat{A}_\mu^{2p}(x) - 2\hat{m}_p \hat{P}^{2p}(x) \right) \hat{O}(y) \right\rangle \Big|_{(R,M)} = \mathcal{O}(a), \quad (\text{A.3})$$

$$\left\langle \left(\partial_\mu^* \hat{A}_\mu^{3p}(x) - 2\hat{m}_p \hat{P}^{3p}(x) + \hat{\epsilon}_p \hat{P}^{0p}(x) \right) \hat{O}(y) \right\rangle \Big|_{(R,M)} = \mathcal{O}(a), \quad (\text{A.4})$$

²¹In particular the symmetry operations that do not leave inert the gauge field must be performed on both quark pairs simultaneously. Important examples of these symmetries are

$$\mathcal{P}_{\pi/2}^1 \times (m_l \rightarrow -m_l) \times (m_h \rightarrow -m_h), \quad \mathcal{P}_F^2 \times (\epsilon_l \rightarrow -\epsilon_l) \times (\epsilon_h \rightarrow -\epsilon_h),$$

with $\mathcal{P}_{\pi/2}^1$ and \mathcal{P}_F^2 representing the obvious extensions of the operations in eqs. (62)–(63) of ref. [4] to the theory with two quark flavour pairs.

where p runs over all possible sea quark pairs present in the theory, $p = \ell, h$. In eqs. (A.3)–(A.4) we have used the definitions

$$\hat{A}_\mu^{2p} = Z_V \bar{\psi}_p \gamma_\mu \gamma_5 \frac{\tau_2}{2} \psi_p, \quad \hat{A}_\mu^{3p} = Z_V \bar{\psi}_p \gamma_\mu \gamma_5 \frac{\tau_3}{2} \psi_p, \quad (\text{A.5})$$

$$\hat{P}^{3p} = Z_P \bar{\psi}_p \frac{\tau_3}{2} \gamma_5 \psi_p, \quad \hat{P}^{0p} = Z_S \bar{\psi}_p \gamma_5 \psi_p, \quad (\text{A.6})$$

and ∂^* is the backward derivative. The above formulae imply the relations

$$\hat{m}_p^+ = \hat{m}_p + \hat{\epsilon}_p = Z_P^{-1} m_p + Z_S^{-1} \epsilon_p, \quad (\text{A.7})$$

$$\hat{m}_p^- = \hat{m}_p - \hat{\epsilon}_p = Z_P^{-1} m_p - Z_S^{-1} \epsilon_p, \quad (\text{A.8})$$

for $p = \ell$ and $p = h$.

The renormalization constants Z_V , Z_P and Z_S are even functions of the Wilson parameter of the quark pair we focus on and the r parameters of all the other sea quark pairs appearing in virtual loops, $Z_I(r_p) = Z_I(r_p; r_\ell, r_h)$, $I = V, P, S, \dots$. The renormalization constants $Z_I(r_p)$ coincide with the corresponding ones of the standard Wilson theory with four flavours, if a mass independent renormalization scheme is employed.

A.2 Valence quark sector

Let us now come to the proof that the valence quark sector of the action (2.1) has the most general renormalizable form compatible with the symmetries of the model.

Due to valence flavour conservation, each valence flavour f renormalizes independently from all the others. Moreover one verifies the validity of the following statements.

1. The $d = 4$ operator $\bar{q}_f \gamma_5 \gamma \cdot \tilde{\nabla} q_f$ is forbidden by \mathcal{C} ;
2. The $d = 3$ operator $i \bar{q}_f \gamma_5 q_f$ can appear with a coefficient (to be identified with the critical mass), proportional to $1/a$ and odd in r_f . Such a term is allowed by the spurionic invariance $\mathcal{P}_5 \times (M \rightarrow -M)$, where

$$\mathcal{P}_5 : \begin{cases} U_0(x) \rightarrow U_0(x_P), & U_k(x) \rightarrow U_k^\dagger(x_P - a\hat{k}), & k = 1, 2, 3 \\ \psi_p(x) \rightarrow \gamma_5 \gamma_0 \psi_p(x_P), & \bar{\psi}_p(x) \rightarrow -\bar{\psi}_p(x_P) \gamma_0 \gamma_5, & p = \ell, h \\ q_f(x) \rightarrow \gamma_5 \gamma_0 q_f(x_P), & \bar{q}_f(x) \rightarrow -\bar{q}_f(x_P) \gamma_0 \gamma_5, & \text{all } f\text{'s} \\ \phi_f(x) \rightarrow \gamma_5 \gamma_0 \phi_f(x_P), & & \text{all } f\text{'s}, \end{cases} \quad (\text{A.9})$$

as such symmetry only excludes coefficients odd in m_f . The spurionic invariance $\mathcal{R}_{5f}^{\text{sp}}$ (see eq. (2.16)) fixes the r_f -parity of the coefficient to be negative. We recall that no odd powers of mass can arise from the sea quark determinant, as the latter is even in the sea quark mass parameters (as well as in the sea Wilson parameters). This proves the statement, made in the text, that the critical mass $M_{\text{cr}}(r_f) = a^{-1} f_{\text{cr}}(r_f; r_\ell, r_h)$ is an odd function of r_f .

3. The $d = 3$ operator $\bar{q}_f q_f$ is allowed, owing to the spurionic invariance $\mathcal{P}_5 \times (M \rightarrow -M)$, only if multiplied by an odd power of m_f (again no odd power of $m_{\ell, h}$ or $\epsilon_{\ell, h}$ can arise from the sea quark determinant). Hence a term like $a^{-1} \bar{q}_f q_f$ is ruled out

and only the term $m_f \bar{q}_f q_f$ needs be included in the action. This implies the multiplicative renormalizability of the valence quark mass parameter, m_f , see eq. (2.7).²² As remarked before, the renormalization constant of m_f , called $Z_m(r_f)$ in the text, must be even in r_f , for consistency with the spurionic invariance $\mathcal{R}_{5f}^{\text{sp}}$.

4. The reality properties of the coefficients of all the quark bilinears are fixed by site/link reflection invariance, $\Theta_{s/l}$. The action of $\Theta_{s/l}$ on gauge and sea quark fields has been specified in eqs. (58)–(59) of ref. [4]. Valence quarks, q_f , and ghosts, ϕ_f , transform under $\Theta_{s/l}$ precisely as each member of the sea quark pair field, ψ_p , while \bar{q}_f transforms as the corresponding antiquark field.

Since we are not interested in correlators with ghost field insertions, we need not discuss in detail the renormalization of the ghost sector of the model. We only wish to stress again that, as we already remarked in the text, the parameters, r_f and m_f , in the ghost action (2.3) are completely fixed by the requirement that integration over the ghost field should exactly cancel the valence fermion determinant.²³

It is also a trivial observation that the invariance of the model (2.1) under independent U(1) transformations acting either on single valence flavours (\mathcal{I}_f , see eq. (2.9)) or individual pairs of sea quarks (\mathcal{I}_p , see eq. (A.2)) guarantees that no fermion bilinears with mixed valence-sea quark content can arise.

As for the operator $iF\tilde{F}$, its presence can be induced neither by integrating over the sea sector [4], because of the invariance under parity (\mathcal{P} , see eq. (2.26)) combined with

$$\psi_{\ell,h}(x) \rightarrow i\tau_3 \psi_{\ell,h}(x), \quad \bar{\psi}_{\ell,h}(x) \rightarrow -\bar{\psi}_{\ell,h}(x) i\tau_3,$$

nor by integrating over the valence sector because the resulting fermionic determinant is exactly canceled by the ghost integration.

We note incidentally that the transformation \mathcal{P}_5 (see eq. (A.9)) can be also cast in the form

$$\mathcal{P}_5 = \mathcal{P} \times \mathcal{R}_{5l} \times \mathcal{R}_{5h} \times \prod_f \mathcal{R}_{5f}, \quad (\text{A.10})$$

where the transformations \mathcal{R}_{5f} and \mathcal{R}_{5p} are defined in eqs. (2.10)–(2.11).

A.3 Sea and valence quark mass renormalization

Here we want to establish the fact that within the model (2.1) a unique dimensionless function, f_{cr} , determines the critical masses in eqs. (2.4)–(2.5) and prove the relation (2.8) between the quark mass renormalization constants of sea and valence quarks.

²²The analysis of chiral WTI's with insertions of valence quark operators leads to the same result.

²³Incidentally if one is willing to consider graded field transformations between valence fermions and ghosts [11], then it turns out that, once the valence fermion action is fixed by the usual renormalization conditions, the form of the ghost action is determined by requiring invariance under e.g. the transformation (with super-determinant equal to 1) $\phi_f(x) \rightarrow q_f(x)$, $q_f(x) \rightarrow \phi_f(x)$, $\phi_f^\dagger(x) \rightarrow \text{sign}(m_f) \bar{q}_f(x)$, $\bar{q}_f(x) \rightarrow \text{sign}(m_f) \phi_f^\dagger(x)$, which for each flavour exchanges quark and ghost fields.

For this purpose, let us consider correlators containing either only the fields ψ_ℓ and $\bar{\psi}_\ell$ or only a pair of valence flavour fields, that we collect in the doublet $Q \equiv (q_1, q_2)$, and choose

$$r_\ell = r_1 = -r_2 \equiv r, \quad m_\ell = m_1 = m_2 \equiv m, \quad \epsilon_\ell = 0. \quad (\text{A.11})$$

In this setting the relation between quark mass renormalization constants we wish to prove reads

$$Z_m(r; r, r_h) = Z_P^{-1}(r; r, r_h). \quad (\text{A.12})$$

It is convenient to consider two pairs of WTI's, one involving correlators made out of exclusively the fields ψ_ℓ and $\bar{\psi}_\ell$ and the second one involving only the valence fields Q and \bar{Q} . The WTI's of interest are ($x \neq y$)

$$\partial_\mu^* \langle V_\mu^{2\ell}(x) P^{2\ell}(y) \rangle \Big|_{(R,M)} = \text{O}(a), \quad (\text{A.13})$$

$$\partial_\mu^* \langle A_\mu^{2\ell}(x) P^{2\ell}(y) \rangle \Big|_{(R,M)} = 2m \langle P^{2\ell}(x) P^{2\ell}(y) \rangle \Big|_{(R,M)} + \text{O}(a), \quad (\text{A.14})$$

where we have used the definitions

$$V_\mu^{2\ell}(x) = \bar{\psi}_\ell(x) \gamma_\mu \frac{\tau_2}{2} \psi_\ell(x), \quad (\text{A.15})$$

$$P^{2\ell}(x) = \bar{\psi}_\ell(x) \gamma_5 \frac{\tau_2}{2} \psi_\ell(x), \quad (\text{A.16})$$

$$\begin{aligned} 2A_\mu^{2\ell}(x) = & \bar{\psi}_\ell(x) \gamma_\mu \gamma_5 \frac{\tau_2}{2} U_\mu(x) \psi_\ell(x + a\hat{\mu}) + \bar{\psi}_\ell(x + a\hat{\mu}) \gamma_\mu \gamma_5 \frac{\tau_2}{2} U_\mu^\dagger(x) \psi_\ell(x) - \\ & - r \left[\bar{\psi}_\ell(x) \frac{\tau_3}{2} U_\mu(x) \psi_\ell(x + a\hat{\mu}) - \bar{\psi}_\ell(x + a\hat{\mu}) \frac{\tau_3}{2} U_\mu^\dagger(x) \psi_\ell(x) \right] \end{aligned} \quad (\text{A.17})$$

and the corresponding WTI's with the ψ_ℓ and $\bar{\psi}_\ell$ fields replaced by the valence fields Q and \bar{Q} , i.e.

$$\partial_\mu^* \langle V_\mu^{2Q}(x) P^{2Q}(y) \rangle \Big|_{(R,M)} = \text{O}(a), \quad (\text{A.18})$$

$$\partial_\mu^* \langle A_\mu^{2Q}(x) P^{2Q}(y) \rangle \Big|_{(R,M)} = 2m \langle P^{2Q}(x) P^{2Q}(y) \rangle \Big|_{(R,M)} + \text{O}(a), \quad (\text{A.19})$$

where analogously we have set

$$V_\mu^{2Q}(x) = \bar{Q}(x) \gamma_\mu \frac{\tau_2}{2} Q(x), \quad (\text{A.20})$$

$$P^{2Q}(x) = \bar{Q}(x) \gamma_5 \frac{\tau_2}{2} Q(x), \quad (\text{A.21})$$

$$\begin{aligned} 2A_\mu^{2Q}(x) = & \bar{Q}(x) \gamma_\mu \gamma_5 \frac{\tau_2}{2} U_\mu(x) Q(x + a\hat{\mu}) + \bar{Q}(x + a\hat{\mu}) \gamma_\mu \gamma_5 \frac{\tau_2}{2} U_\mu^\dagger(x) Q(x) + \\ & + r \left[\bar{Q}(x) \frac{\tau_1}{2} U_\mu(x) Q(x + a\hat{\mu}) - \bar{Q}(x + a\hat{\mu}) \frac{\tau_1}{2} U_\mu^\dagger(x) Q(x) \right]. \end{aligned} \quad (\text{A.22})$$

Imposing the validity of the WTI's (A.13) and (A.18) is a way of arriving at a definition of the critical mass for the light quark pair and the valence quark doublet $Q = (q_1, q_2)$, respectively. The key observation is that, with the choice (A.11) of bare parameters, the l.h.s. of eq. (A.13) is exactly equal to the l.h.s. of eq. (A.18). To prove this it is enough

to perform a (suitable) vector- τ_2 rotation of the ℓ ight quark field pair, so as to rewrite its action in the basis where the Wilson term is multiplied by $-i\gamma_5\tau_3$ as is the case of the Q -doublet. Such a rotation does not alter the expression of the operators (A.15) and (A.16), but brings the flavour structure of the axial current (A.17) to that of eq. (A.22). It thus follows that the numerical value of $M_{\text{cr}} = a^{-1}f_{\text{cr}}(r; r, r_h)$ inferred by enforcing the vanishing of the r.h.s. of eq. (A.13) is the same that is obtained by enforcing the same condition on eq. (A.18), and viceversa. This proves the relations (2.4)–(2.5).

The WTI's (A.14) and (A.19) contain all the relevant information about the quark mass of the ℓ ight quark pair and the valence quark doublet (q_1, q_2) , respectively. Moreover they involve the exactly conserved 1-point split axial currents (A.17) and (A.22). Precisely for this reason, the quark mass renormalization factor can be taken equal to the inverse of the renormalization constant of the relevant pseudo-scalar densities, which are $P^{2\ell}$ (eq. (A.16)) and P^{2Q} (eq. (A.21)) for the ℓ ight quark pair and the valence quark doublet, respectively. In the text we have denoted the mass renormalization constant of the ℓ ight quark pair by $Z_P^{-1}(r) = Z_P^{-1}(r; r, r_h)$ and that of the valence fields $Q = (q_1, q_2)$ by $Z_m(r) = Z_m(r; r, r_h)$ (recall that Z_m is even in r and we have taken $r_1 = -r_2 \equiv r$, see eq. (A.11)). At this point the relation (A.12) is a consequence of the fact that, by the same argument we gave before for the vector WTI's (A.13) and (A.18), the correlator $\langle P^{2\ell}(x)P^{2\ell}(y) \rangle|_{(R,M)}$ in eq. (A.14) is equal to the correlator $\langle P^{2Q}(x)P^{2Q}(y) \rangle|_{(R,M)}$ in eq. (A.19).

B. Isospin and parity breaking effects in the light quark sector

Although to guarantee the desired renormalization properties of Q_{VA+AV}^\pm only the condition $|r_u| = |r_d|$ is actually necessary, the choice (4.17) is quite convenient as it preserves (for $m_d = m_u$) the isospin symmetry of the action of the u and d pair of valence quarks. As a consequence of this symmetry, the two-pion states $|\pi^+\pi^- \rangle$ and $|\pi^0\pi^0 \rangle$ cannot mix with the neutral pion state, $|\pi^0 \rangle$, as it would be the case had we chosen the condition $r_u = -r_d$ instead of (4.17). This remark is very important in practice, because (recall that parity is not a symmetry of tm-LQCD) it allows to exclude the presence of the neutral pion state among the low mass states contributing to the spectral representation of the correlators $C_{\pm, \pi^+\pi^-}^{(4s10v)}(x, z, y)$ and $C_{\pm, \pi^0\pi^0}^{(4s10v)}(x, z, y)$ (see eqs. (4.9)–(4.10)).

It should be noted, in fact, that, if present (as in the case isospin is broken by the choice $r_u = -r_d$ or by taking $m_d \neq m_u$), the contribution of the neutral pion may numerically compete with the relevant isospin and parity preserving contributions, since its mass is generically lower than the energy of the two pion states we are interested in. Consistently with the general properties of tm-LCDQ it can, however, be shown that isospin and parity breaking contributions to the spectral representation are mere $O(a^2)$ cut-off effects. The latter can be disentangled by standard techniques and removed from the measured correlators before extracting the relevant $O(1)$ contributions.

There is an extra problem that should be mentioned if isospin (and parity) is broken. Namely the fact that the standard interpolating field for the neutral pion, eq. (4.22), mixes with the identity operator. To avoid this problem one may replace the latter with the

fourth component of the neutral axial current

$$\Phi_{\pi^0} = \Phi_{\pi^0}^\dagger \rightarrow \frac{1}{\sqrt{2}} \left[\bar{u} \gamma_0 \gamma_5 u - \bar{d} \gamma_0 \gamma_5 d \right].$$

C. Absence of the mixing of \mathcal{Q}_{VA+AV}^\pm with operators of dimension six

In this appendix we prove that the operators $\mathcal{Q}_{VA+AV}^{\pm[k]}$ cannot mix with any other operator of dimension six. Looking at eqs. (4.16)–(4.17), we see that just two operators need to be considered, i.e.

1. $\mathcal{Q}_{VA+AV}^{\pm[0]}$, where valence quark species have $r_u = r_c = r_d = r_s$;
2. $\mathcal{Q}_{VA+AV}^{\pm[1]}$, where valence quark species have $r_{u'} = r_{c'} = -r_d = -r_s$.

Indeed the case of $\mathcal{Q}_{VA+AV}^{\pm[2]}$ is identical to the case of $\mathcal{Q}_{VA+AV}^{\pm[0]}$, and the case of $\mathcal{Q}_{VA+AV}^{\pm[3]}$ to that of $\mathcal{Q}_{VA+AV}^{\pm[1]}$, because the quarks that enter have an equal pattern of signs of the Wilson parameters.²⁴

Since we are discussing the mixing of operators of the same dimension, we can set to zero the masses of the quarks and consider the lattice model $(4s10v)_{tm}^L$ in the chiral limit.

Let us discuss separately the case of $\mathcal{Q}_{VA+AV}^{\pm[0]}$ and $\mathcal{Q}_{VA+AV}^{\pm[1]}$.

C.1 The operator $\mathcal{Q}_{VA+AV}^{\pm[0]}$

A basis for the operators of dimension six which $\mathcal{Q}_{VA+AV}^{\pm[0]}$ can mix with is given by [20]

$$\begin{aligned} & \mathcal{Q}_Y^{+[0]}, \quad \mathcal{Q}_Y^{-[0]}, \\ & Y = VA + AV, VA - AV, SP + PS, SP - PS, T\tilde{T}, \\ & VV + AA, VV - AA, SS + PP, SS - PP, TT. \end{aligned} \quad (C.1)$$

The notation $VA + AV, VA - AV, \dots, TT$ refers to the Dirac structure of the four-fermion operators and is self-explanatory. For instance, with $\sigma_{\mu\nu} \equiv i[\gamma_\mu, \gamma_\nu]/2$, we have

$$\begin{aligned} \mathcal{Q}_{VV+AA}^{\pm[0]} &= \frac{1}{2} \left[(\bar{s} \gamma_\mu u)(\bar{u} \gamma_\mu d) \pm (\bar{s} \gamma_\mu d)(\bar{u} \gamma_\mu u) \right] - \frac{1}{2} [u \leftrightarrow c] + \\ &+ \frac{1}{2} \left[(\bar{s} \gamma_\mu \gamma_5 u)(\bar{u} \gamma_\mu \gamma_5 d) \pm (\bar{s} \gamma_\mu \gamma_5 d)(\bar{u} \gamma_\mu \gamma_5 u) \right] - \frac{1}{2} [u \leftrightarrow c], \end{aligned} \quad (C.2)$$

$$\mathcal{Q}_{TT}^{\pm[0]} = \frac{1}{2} \left[(\bar{s} \sigma_{\mu\nu} u)(\bar{u} \sigma_{\mu\nu} d) \pm (\bar{s} \sigma_{\mu\nu} d)(\bar{u} \sigma_{\mu\nu} u) \right] - \frac{1}{2} [u \leftrightarrow c]. \quad (C.3)$$

The key observation is that, owing to the equality $r_u = r_c = r_d = r_s$ of the Wilson parameters of the quarks appearing in $\mathcal{Q}_Y^{\pm[0]}$, the part of the lattice action relative to these quarks (the standard u, d, s and c quarks) admits an exact $SU(4)$ flavour symmetry,

²⁴The arguments that follow would go through also if we were to replace eq. (4.17) with $r_u = -r_d$, while maintaining eq. (4.16). In fact, this new choice for the valence Wilson parameters is related to the one we made in the text by the transformation $\text{Ex}(u, u') \times \text{Ex}(u'', u''') \times \text{Ex}(c, c') \times \text{Ex}(c'', c''')$ which leaves invariant the form of the operator \mathcal{Q}_{VA+AV}^\pm . See, however, appendix B.

which prevents the operators of the type (+) to mix with any of the (−) counterparts, as they belong to different irreducible representations of the SU(4) flavour group. The operators in (C.1) can be thus viewed to yield two separate bases, one for the (+) sector and another one for the (−) sector, containing the candidates for the mixing with $\mathcal{Q}_{VA+AV}^{+[0]}$ and $\mathcal{Q}_{VA+AV}^{-[0]}$, respectively.

Notice that conservation of each separate valence quark species forbids the mixing of the operators $\mathcal{Q}_{VA+AV}^{\pm[0]}$ with the operators $\mathcal{Q}_Y^{\pm[k]}$, $k = 1, 2, 3$, as they have different flavour content.²⁵

For brevity, we will deal “in parallel” with $\mathcal{Q}_{VA+AV}^{+[0]}$ and $\mathcal{Q}_{VA+AV}^{-[0]}$. One checks that the invariance of the action $(4s10v)_{tm}^L$ under \mathcal{P}_5 (see eq. (A.9)) rules out the mixing of $\mathcal{Q}_{VA+AV}^{\pm[0]}$ with the operators of the form $\mathcal{Q}_W^{\pm[0]}$, having the Dirac structure $W = VV + AA, VV - AA, SS + PP, SS - PP, TT$. In fact, these operators are even under \mathcal{P}_5 , while $\mathcal{Q}_{VA+AV}^{\pm[0]}$ is odd.

To complete the proof we notice that under the symmetry transformation $\text{Ex}(d, s) \times \mathcal{C}$, the operator $\mathcal{Q}_{VA+AV}^{\pm[0]}$ is odd, while the operators $\mathcal{Q}_{SP+PS}^{\pm[0]}$ and $\mathcal{Q}_{T\tilde{T}}^{\pm[0]}$ are even. As for the operators $\mathcal{Q}_{VA-AV}^{\pm[0]}$ and $\mathcal{Q}_{SP-PS}^{\pm[0]}$ they have more complicated transformation properties, namely $\mathcal{Q}_{VA-AV}^{\pm[0]} \rightarrow \mathcal{Q}_{VA-AV}^{\mp[0]}$ and $\mathcal{Q}_{SP-PS}^{\pm[0]} \rightarrow -\mathcal{Q}_{SP-PS}^{\mp[0]}$. The operators that under $\text{Ex}(d, s) \times \mathcal{C}$ have the same transformation properties as $\mathcal{Q}_{VA+AV}^{\pm[0]}$ are thus the combinations $\mathcal{Q}_{VA-AV}^{+[0]} - \mathcal{Q}_{VA-AV}^{-[0]}$ and $\mathcal{Q}_{SP-PS}^{+[0]} + \mathcal{Q}_{SP-PS}^{-[0]}$, but SU(4) flavour symmetry prevents $\mathcal{Q}_{VA+AV}^{\pm[0]}$ from mixing with them. This concludes the proof for $\mathcal{Q}_{VA+AV}^{\pm[0]}$.

C.2 The operator $\mathcal{Q}_{VA+AV}^{\pm[1]}$

We now consider the case of the operator $\mathcal{Q}_{VA+AV}^{\pm[1]}$, which differs from the previous one only because the Wilson parameters of the relevant valence quarks obey the relation $r_{u'} = -r_d = -r_s = r_{c'}$.

The mixing and renormalization properties of the operator $\mathcal{Q}_{VA+AV}^{\pm[1]}$ can be brought back to that of the operator $\mathcal{Q}_{VA+AV}^{\pm[0]}$, discussed above, by simply observing that the change of functional integration variables induced by the transformation $\mathcal{R}_{5u'} \times \mathcal{R}_{5c'}$ does not touch the expression of $\mathcal{Q}_{VA+AV}^{\pm[1]}$ and leaves invariant the massless action of the valence quarks, apart from switching the signs of the Wilson terms of the quark species u' and c' . We get in this way precisely the situation we had before. Since a change of variable in the functional integral leaves unchanged all the correlators, from the absence of mixing we proved in the case of $\mathcal{Q}_{VA+AV}^{\pm[0]}$ we can infer the same result for $\mathcal{Q}_{VA+AV}^{\pm[1]}$. This ends the proof.

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²⁵Of course, away from the chiral limit each of the $\mathcal{Q}_Y^{\pm[k]}$, $k = 0, 1, 2, 3$ can mix with $\Delta s = -\Delta d = 1$ two-quark operators having the same unbroken quantum numbers, as we discussed in the text.

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